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APPLIED MATHEMATICAL WATER-QUALITY MODELING OF SHELF MARINE ECOSYSTEMS

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We present the results of investigation of the present-day ecological state of shelf marine ecosystems subjected to strong anthropogenic load and evaluate actual possibilities of control of their water quality by using methods of numerical mathematical modeling of natural processes in marine medium.
The proposed model is used as a tool for the prediction of ecological consequences and the assessment of the appropriateness and efficiency of various administrative solutions aimed at the preservation and improvement of the water quality of the investigated water objects.
The monograph is intended for administrative institutions, research and engineering institutes, and natural-sciences departments of universities.

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INTRODUCTION

The growth of population of the Earth and the scientific and technological progress resulted in the escalation of anthropogenic impact on the environment. At present, the anthropogenic load on the biosphere is not only commensurable with natural processes and cycles, but, in many cases, excel them and exceed the self-restoring capabilities and properties of natural ecosystems. This leads to irreversible consequences for natural and anthropogenic systems.

The most important component of natural environment is the hydrosphere, more than 97% of it being the World Ocean. In the nearest future, the mankind will have to solve problems related to the exhaustion of reserves of many natural resources of dry land, and, therefore, the significance of the World Ocean as a source of huge reserves of mineral, energy, and biological resources will grow.

The expansion of the sphere of human activity in the oceans and seas occurs, first of all, in the shelf regions, which are the most productive area of the World Ocean. The capacity of the biomass of littoral regions of the ocean exceeds the capacity of dry land by more than two orders of magnitude [61]. At present, the most part of biological and mineral resources of the sea is extracted exactly in the shelf areas. The development of these resources is accompanied by an increase in the anthropogenic impact on marine ecosystems, which threatens their existence itself.

The anthropogenic impact on the ecosystems of sea shelf areas is not limited by the use of their resources. As a result of industrial and household human activity, a huge amount of various pollutants gets into the littoral areas of the sea with river waters and sewage. Numerous substances that are used or manufactured on dry land as a result of human activity are eventually discharged to the sea and accumulated in its shelf area.

The increasing anthropogenic load on the littoral areas of the sea leads to the violation of the existing balance of processes and degradation, and overrange of admissible ecological niches of shelf ecosystems, which, in turn, leads to stable changes in the structure and functioning of marine biocenoses and, in some cases, to their complete disappearance. In this connection, the problem of control of the quality of littoral sea waters by means of the regulation and optimization of the discharge of pollutants, the realization of various ecologically oriented waterworks projects, etc., becomes especially urgent.

The objective scientifically substantiated prediction of ecological consequences of the impact of existing and planned economic objects on the marine medium and the evaluation of the efficiency of various administrative decisions in the field of rational use, protection, and restoration of resources of the sea shelf area are impossible without using mathematical models, combined under the common name of "water-quality models." The development and verification of such mathematical models intended for using as a tool of ecological prediction in the course of scenario modeling of natural processes is one of the main aims of ecological monitoring of littoral sea areas.

The appropriateness and necessity of the application of mathematical models to the solution of problems related to the development of a strategy for control of the quality of water medium are explained by the fact that such models enable one to take into account, in decision making, the correlation of the components of an ecosystem and the possible "counterintuitiveness" of its behavior under changes in external loads, thus moving ecological predictions from the category of intuitive predictions into the category of objective ones.

Due to the active development and utilization of resources of the Ukrainian sea shelf, of special importance is the problem of preservation and improvement of quality of marine medium, guaranteeing of ecological safety, and minimization of damage caused by human economic activity to the ecosystems of littoral and shelf areas of the Black and Azov Seas. The solution of these problems requires applied water-quality models that combining such properties as complexity, informativeness, and adequacy to natural analogs with the minimization of costs for their adaptation, calibration, and practical realization. The broad application of these models to the solution of applied problems of sea ecology is impossible without their information support, calibration, and practical use for the development of scientifically substantiated recommendations on the preservation and improvement of quality of water medium and its resources.

In the present work, we generalize our experience in the development and use of numerical mathematical water-quality models for the solution of applied ecological problems and the determination of optimal strategy of control of water quality in shelf marine ecosystems at tropical and temperate latitudes subject to strong anthropogenic impact.

The objects of investigation in this work are shelf marine ecosystems of littoral sea basins of the Colombian coast of the Caribbean Sea and the northwest part of the Black Sea, or, more specifically, the quality of water in these ecosystems. On the basis of data of monitoring, we carry out an ecosystem analysis of the present-day ecological state of tropical sea basins of the Colombian coast of the Caribbean Sea. We obtain new information on operating hydrochemical characteristics of Odessa region of the northwest part of the Black Sea and their relation to river discharge, hydrological conditions and phenomena, and the operation of anthropogenic pollution sources in the littoral area. We also describe the ecological consequences of anthropogenic action on the ecosystems of the investigated marine water areas.

On the basis of investigations of specific features of eutrophication of waters in the sea shelf areas at temperate and tropical latitudes, we develop a new nonstationary applied numerical water-quality model and its different modifications. We propose original schemes and methods for the calibration of eutrophication blocks of the water-quality model, which were successfully tested and showed their efficiency in the solution of applied problems for marine water areas and basins belonging to different climatic zones and having different morphological, hydrological, hydrochemical, and hydrobiological characteristics.

We develop requirements to the organization and structure of ecological monitoring of marine medium, including specialized experiments motivated by the necessity of information support of the development, adaptation, calibration, and use of water-quality models for the solution of practical problems of sea ecology. We determine, generalize, and systematize methodological approaches to the determination of parameters of water-quality models on the basis of results of ecological monitoring. We also generalize and systematize the results of different investigations for the the determination of the characteristic values of the rates of chemical and biological processes, which are taken into account in water-quality models for marine and fresh-water ecosystems, the ranges of their variability, and dependences on characteristics of water medium.

The proposed model is used as a tool for the prediction of ecological consequences and the evaluation of the appropriateness and efficiency of various administrative decisions aimed at the preservation and improvement of water quality of the investigated water objects. We develop and improve the methodology of application of numerical mathematical models to the determination of the optimal strategy of control of water quality in shelf marine ecosystems subject to strong anthropogenic load. For the investigated marine water areas, using results of numerical simulation experiments with modifications of the model, we determine optimal strategies for the realization of nature-conservation measures aimed at the improvement of water quality in these basins.

The results that form the basis of this work were obtained within the framework of 11 national and international projects that were carried out at the Odessa Branch of the Institute of Biology of Southern Seas of the Ukrainian National Academy of Sciences, the Centro de Investigaciones Oceanográficas e Hidrográficas (Colombia), and the Odessa State Ecological University.

We are grateful for fruitful cooperation to all our colleagues—the coauthors of publications from the Marine Hydrophysical Institute of the Ukrainian National Academy of Sciences, the Odessa Branch of the Institute of Biology of Southern Seas of the Ukrainian National Academy of Sciences, the Odessa State Ecological University, and the Centro de Investigaciones Oceanográficas e Hidrográficas (Colombia). We want to especially acknowledge our many-year collaboration with S. A. Lonin, a Candidate of Physical and Mathematical Sciences, who now continues his scientific work in Colombia, and O. Yu. Sapko, an assistant-lecturer of the Department of Ecological Law at the Odessa State Ecological University, whose materials were used in the preparation of Sections 2.2.1 and 7.3.

1. ROLE OF MATHEMATICAL MODELING IN THE SOLUTION OF THE PROBLEMS OF QUALITY CONTROL FOR WATERS OF THE ECOSYSTEMS OF SEA SHELF

In what follows, the quality of seawater is regarded as a characteristic of its composition and properties specifying the turnover of substances, bioproductivity, structure and regularities of functioning of a marine ecosystem, its ecological state, and suitability for various kinds of water consumption. Since the quality of marine media is evaluated, first of all, from the viewpoint of guaranteeing of the optimal conditions for the reproduction of biological resources of the sea and vital activity of human beings, the concept of quality of the habitat is closely connected with the notion of ecosystem. An ecosystem (biogeocenosis) is defined as a space system including a historically formed complex of living organisms (biotic components) connected by trophic links and lifeless (abiotic) components of the habitat used in the processes of metabolism and energy exchange.

Any marine ecosystem is, in fact, a complex, multicomponent biogeothermodynamic system whose functioning is determined by a complex of correlated phenomena and processes of physical, chemical, and biological nature. The biotic and abiotic components of the ecosystem are connected by complex relationships with positive and negative feedback. As a result of the interaction of these components realized via numerous fairly weak mechanisms, the ecosystem is kept in the state of dynamic equilibrium or is close to this state. The entire ecosystem is characterized by the presence of certain specific properties that are not exhibited by its separate components.

As an important consequence of the complexity of marine ecosystems, we can mention their "counterintuitive" behavior in response to the anthropogenic actions in the cases where, at first sight, favorable and efficient decisions led to absolutely unexpected consequences. Therefore, in order to predict more or less correctly the ecological consequences of making administrative decisions, it is necessary to apply the corresponding procedures based on the principles of systems analysis. For this purpose, one can use the methods of mathematical modeling of the operation of marine ecological systems.

As a rule, prior to the creation of a mathematical model, it is reasonable to perform the ecological monitoring of the analyzed ecosystem and a series of specialized experiments aimed at the evaluation of the intensity of links between the components of the ecosystem. In view of the complexity of links in natural ecosystems and correlations between them, it is, in principle, impossible to realize complex synchronous observations over the components of an ecosystem and the processes connecting these components with sufficiently high space and time resolution. The *in-situ* observations are performed by large groups of different experts with narrow scientific specializations on the basis of the available methods, at different times and points of the space, and for different combinations of the factors affecting the observed parameter or process. As a result, in the course of generalization and systems analysis of these data, it is often discovered that the average statistical values of some characteristics specifying the state of the ecosystem are incompatible or even incomparable. Hence, the construction of the models of ecosystems can be regarded as an important tool used for the verification of the compatibility of separate facts and the data of observations established in the course of the *in-situ* investigations and experimentally. These models enable us to combine and reflect (on a common formal basis) the existing ideas concerning the key factors and principal mechanisms determining the specific features of functioning of the actual ecosystems, estimate the adequacy of some results of the field and laboratory modeling, and analyze different scientific hypotheses within the framework of a single model.

The process of development of a model and numerical experiments with it include, to a significant extent, the analysis of functioning of an ecosystem and, hence, lead to the better understanding of the system. The mathematical models enable one to reveal the genetic relations in the dynamics trends of the components of the ecosystem and its state as a whole, to study the space-and-time variability of the components depending on the external factors, and to give comparative estimates of the roles of various natural and anthropogenic factors in the formation of the quality of waters and the specific features of functioning of the ecosystem. The application of the models also enables one to estimate the interactions formed in the actual systems that cannot (or almost cannot) be investigated by direct measurements. By using the results of modeling, one can optimize the program of ecological monitoring.

The anthropogenic actions upon the marine media depend on the decisions made in the field of economical activity: on the construction of new objects, expansion of the existing structures, and transition to the new technologies of production of the resources. The realization of the engineering projects cannot be performed by the trial-and-error method. It is always necessary to be able to predict possible consequences of this kind of activities [5]. This problem is solved on the basis of the application of the methods of mathematical modeling of complex natural systems.

In the ecological investigations, the mathematical models are mainly used to estimate the influence of various types of anthropogenic actions upon the ecosystems because this can be done much faster and cost efficiently than in the actual natural systems and without any risk of negative unexpected effects with (sometimes) irreversible consequences.

At present, numerical simulation is the most promising procedure of mathematical modeling of natural ecosystems. In the process of simulation, the applied mathematical model reproduces the algorithm ("logic") of functioning of the analyzed system in time for various combinations of the values of the parameters of the system and the environment.

The process of operation of any system can be formally described by using the following variables:

(i) *variables of state,* i.e., quantitative parameters of the system representing certain generalized characteristics of its state and characterizing the mode of its operation; in the case of marine ecosystems, the collection of these parameters includes, e.g., the biomass, the concentration of biogenic substances, etc.;

(ii) *input variables,* i.e., the variables reflecting the influence of the environment on the system (external factors), e.g., the hydrometeorological conditions, discharges of pollutants, etc.; among these variables, we distinguish the components caused solely by the natural factors and the components regulated, to a certain extent, by the society; the last group includes the anthropogenic factors often called control variables;

(iii) *output variables,* i.e., the variables characterizing the response of the system to the action of the environment; these parameters can either form a subset of the variables of state or include the quantities computed as functions of the variables of state.

By changing the control variables within the actual or predicted ranges of their variability and performing the mathematical simulation of an ecosystem, the researcher can analyze the degree of anthropogenic influence upon its operation and structure and the possibility of control over the ecosystem. One of the main aims of mathematical simulation is to get various sets of solutions corresponding to the systematically changed initial data, i.e., to perform the numerical experiments with the model instead of risky and often impossible *in-situ* experiments with the nature [80].

The mathematical models play the role of an efficient tool for the prediction of the consequences of anthropogenic influence upon the state of ecological systems. The predictions of the trends of changes in the state of an ecosystem obtained according to the results of simulation enable us to take into account possible consequences of the implementation of various economical programs and determine scientifically substantiated complex plans of nature-preservation measures [5].

If it is desirable to control the system with an aim to get a certain result, then the simulation model can be used to check all possible combinations of the existing strategies of control (with minimum amounts of efforts and costs spent for this purpose) and, hence, to find the desired optimum [59]. In this case, we not only predict the ecological consequences of various kinds of anthropogenic influence upon the ecosystem but also determine the ways of minimization of damage caused to the environment. The procedure of mathematical simulation is characterized by high practical possibilities as for the control over the natural resources and can be regarded as the principal tool for the evaluation of the efficiency of the alternative strategies of utilization of natural resources and making decisions optimal from the viewpoint of nature preservation.

Thus, the mathematical models play the role of a link between the ecological theory, scientific investigations, and management. With the help of the systems analysis, one can combine the data and information obtained in numerous investigations into a single interrelated model. The solution of the system of differential equations gives a prediction of the response of the ecosystem to external actions. On the other hand, it might be possible to determine a set of actions promoting, in a certain sense, the optimal response of the ecosystem in agreement with the restrictions imposed on the available methods of control [59].

Thus, the general aim of mathematical modeling in the process of management (decision making) can be formulated as follows: To determine (compute) the values of the chosen parameter of efficiency of a decision for various strategies of realization of an operation (ways of realization of a project). In the process of development of a specific model, the aim of modeling should be made more precise with regard for the chosen criterion of efficiency of the decision. As for the criterion of applicability, the model should guarantee the possibility of finding the values of the parameter of efficiency for the entire set of the admissible strategies. The criterion of optimality should enable us to determine the parameters of the analyzed object corresponding to the extreme values of the parameter of efficiency of decisions directly by using the model [25].

Among the problems of control over the ecological systems of shelf regions of the sea, the principal role is played by the problem of control over the quality of water under the conditions of action of pollutants of the anthropogenic origin because the possibility of prediction of the quality of water is of fundamental importance for the prediction of the other properties of the ecosystem, e.g., its bioproductivity.

1.1. Principles of Construction of the Complex Models of Functioning and Dynamics of Water Ecosystems

For the analysis of the actual information possibilities and correct and efficient practical application of the numerical mathematical models of functioning of the marine ecosystems and the formation of the quality of seawater, it is necessary to know their general structure, the chemical and biological processes included in the model, and the applied generalizations, approximations, and simplifying hypotheses.

At present, there exist numerous models of marine systems characterized by different degrees of complexity. In this collection, it is necessary to indicate the specific features of the class of models of the quality of water and estimate the level of their development and information possibilities connected with the solution of applied problems of the ecology of sea.

Actual water ecosystems are characterized by the presence of thousands simultaneously running correlated processes described by the corresponding systems of equations. These complex systems cannot be solved numerically. Furthermore, even in the case where the solution of a system of this sort is somehow obtained, the corresponding results would not be precise and could not be analyzed due to the inaccuracy of the equations in this system and the coefficients appearing in these equations.

Hence, in constructing the models of water ecosystems, it is necessary to use the *hierarchical principle* of taking into account the processes running in the ecosystem. According to this principle, in the initial stages of modeling, we use a simplified version of the model reflecting, with a sufficient degree of accuracy, the variability only of the most important components of the ecosystem and the processes connecting these components, i.e., the components without which it is impossible to give a reliable description of the actual ecological situations and, thus, realize the main aim of modeling. These models can easily be calibrated and verified and the results of their application can be unambiguously interpreted in terms of genetic relations.

The hierarchical principle in the structure and analysis of the models of complex systems is based on the objectively existing hierarchy of natural processes, their distribution over space-and-time scales and the contribution to the final state of the system for its descriptions performed with different degrees of going into detail [5].

The realization of the hierarchical approach to the development of the models of functioning of ecosystems is based on the application of the principles of *aggregation* and space-and-time *averaging* of modeled components of the actual ecosystem with subsequent hierarchical decomposition.

In the initial stages of modeling, the structural description of biocenosis is realized by the organization of the organisms into ecological trophic groups containing the organisms with similar ecological, trophic, and physiological characteristics (e.g., phytoplankton, bacteria, zooplankton, etc). The procedure of aggregation can also be performed according to the intensity of metabolism of the organisms or according to their sizes (in view of the fact that, in the pelagic communities, larger organisms usually eat smaller creatures) [65]. Both these approaches can be combined and then the procedure of selection of the biotic elements of the ecosystem (components of the model) is realized according to ecological trophic groups with regard for the size classes of organisms.

In describing the inert organic matter as one of the most important bioinert elements of the ecosystem, it is possible to neglect, in the simplest case, its separation into the dissolved and suspended (or into the labile and poorly oxidized) fractions.

In the process of accumulation and improvement of information about the variability of elements of the ecosystem and the processes and factors responsible for the indicated variability, it is necessary to perform the *decomposition* of components of the model, e.g., to consider (in the subsequent stages of modeling) different groups of the system or size groups of phytoplankton instead of the variations of the biomass of phytoplankton as a single aggregated autotrophic element of the ecosystem. The entire collection of zooplankton can also be split into microzooplankton, predatory, and nonpredatory mesozooplankton, etc.

In agreement with the principles of averaging, the models may have different space-and-time resolutions. The calibration and operation of three-dimensional prognostic models of water ecosystem require quite high productivity of the computers and significant (often unrealistically large) amounts of computer time and efforts of the researchers. Hence, in the initial version, the models are usually of dimensionality zero (averaged over the space) or one-dimensional (with resolution over the vertical coordinate). Only after their calibration and verification, it is possible to proceed to the realization of the three-dimensional version of the model accompanied by the correction of the already established parameters and the coefficients of the model.

The time step of the model depends on the aims of modeling and the specific features of variability of the components of the ecosystem and the factors specifying these components. In most cases, the hydrological, chemical, and biological processes in the actual ecosystems are characterized by different scales of variability in time and, therefore, by different time steps used in their modeling.

Depending on the purposes of modeling and the specific features of the water ecosystem, the variability of its chemical and biological components can also be described with different time steps. Thus, if it is necessary to reflect in the model some specific features of the seasonal course of elements of the water ecosystem at middle latitudes, then the step of the model is set equal to one day, which enables one to neglect the inertia of the processes of feeding and photosynthesis and, at the same time, average the fluctuations of the distributions caused by the vertical migrations. However, in the tidal seas of tropical latitudes, where the seasonal variability of some chemical and biological elements of the ecosystem is comparable with their daily variability, the analysis of the daily variations of the rate of photosynthesis is of principal importance for the correct solution of the problem.

In constructing the mathematical models of water ecosystems, it is also customary to use an important principle of *parametrization* of some processes and the possibility of neglecting, in the first approximation, some feedbacks introduced in the subsequent stages of modeling of the system. As a rule, this principle is applied for the description of the processes and links in the ecosystem whose mechanisms are studied insufficiently well or the required information is absent. Thus, in describing the processes of nitrification or biochemical oxidation of the inert organic matte determined, in fact, by the metabolism of bacteria, the rates of the corresponding processes are taken into account but the indicated bacteria are most often not included in the model as an element of the ecosystem.

If the model does not describe the principal features of operation of the ecosystem, then it is necessary to make some of its blocks more complicated and include additional elements of the ecosystem (and the processes responsible for their variability) in the model, i.e., in this case, we use the principle of *decomposition.* In the solution of practical problems of utilization of the marine resources, the application of more complex structures of ecological models is reasonable only in the case where it is necessary to guarantee the possibility of adequate reflection in the model of the required observed properties of the ecosystem and the dynamics of its components that cannot be described by using simpler models.

The second important condition of adequacy and efficiency of the model is the completeness of scientific knowledge about the variability of modeled elements of the ecosystem and the corresponding processes.

As indicated in [65], the sizes and complexity of the model should be determined by the posed problem. Thus, on the one hand, the smaller the number of elements of the ecosystem included in the model, the rougher and less exactly the actual picture is reflected by the processes described by the model. However, on the other hand, in the case where the amount of reliable information on the processes running in the ecosystem is insufficient, the application of more detailed versions of the model does not always lead to the improvement of the results because, in this case, the number of degrees of freedom in the process of calibration of the model according to the data of observations increases and the analysis of the genetic relations in the obtained solution and, hence, the verification of the model and interpretation of the accumulated results become more complicated. Contrary to the expectations, the prognostic properties of the model can become even worse. This is explained by the fact that the current level of knowledge enables us to give sufficiently exact descriptions and/or predictions solely for the biological phenomena determined by the physical and chemical processes. At the same time, if the key role is played by the processes of pure biological nature, then the procedure of prediction becomes much more complicated. Moreover, the fluxes of substance and energy between the components of the ecosystem are often described in the models by nonlinear empirical relations, which leads to serious mathematical difficulties connected with the ambiguity and bifurcations of the solutions obtained as a result. These difficulties become much more pronounced as the number of equations used to describe the behavior of the biocenosis increases.

Thus, the most important stage of modeling is connected with the reduction of the number of modeled variables and analyzed processes (depending on the aim of modeling) and the choice of procedure of integration of interactions between the elements of the system [18]. In each case, it is reasonable to be fairly careful in choosing the level of complexity of the created model and select its optimal version for every posed problem. The structure of the model is regarded as sufficient if it enables one to solve the required problems and gives an adequate description of the actual processes running in the ecosystem. The mathematical foundations of the model should be constructed to guarantee the principal possibility of evaluation of the parameters appearing in the equations as a result of the experimental investigations or *in-situ* observations [65].

There exist different kinds of links between the elements of marine biocenoses: trophic, topical, symbiotic, and metabolic. However, the data of ecological investigations show that the principal role in the formation of any ecological community as a single system (specifying the basis of its structure and productivity) is played by the food (trophic) links [65]. Therefore, the principal biological processes taken into account in the models of ecosystems are the processes of transformation of substances and energy in passing through the trophic chains. The process of transfer of substances and/or energy from one element of the ecosystem to another connected with their transformations is called a flux. As an example, we can mention the absorption of biogenic substances in the process of generation of primary production, eating of a certain type of organisms by the other organisms, mineralization of the inert organic matter, etc. Parallel with the fluxes of substance and energy between the elements of a system, the water media are also characterized by their spatial redistribution caused by the hydrodynamic processes (advective transfer, turbulent mixing, and dispersion).

In constructing the models of ecosystems, the role of biotic elements of the ecosystem is played not by the separate organisms but by the organic matter contained in the populations. The amount of this matter is, as a rule, quantitatively evaluated as the biomass expressed in the units of content of the most widespread biogenic elements circulating in the ecosystem (carbon, nitrogen, and phosphorus) or via the energy flowing through the system. The application of biogenic elements as a standard measure proves to be very convenient in view of the fact that just the fluxes of these elements combine the abiotic and biotic elements of the ecosystem into a single whole. In most models, it is customary to use the assumption that the chemical composition of organic matter is constant and corresponds to its stoichiometric model $(CH_2O)_{106}(NH_3)_{16}H_3PO_4$ [3], i.e., the ratio of the amounts of carbon, nitrogen, and phosphorus in the organic matter $C:N:P = 106:16:1$ in micromoles or $41:7.2:1$ in mass units.

The principal method used for the mathematical description of the dynamics of marine ecosystems with regard for the entire complex of combined physical, chemical and biological processes is connected with the solution of a system of differential equations deduced for the description of the variability of biogeocenoses. The number of equations in this system must be equal to the number of the variables of state of the ecosystem, i.e., the mathematical system must be closed.

As the mathematical tool for the description of interaction between the hydrodynamic processes of mass transfer in the three-dimensional space and the chemical and biological processes of translocation of substances on a common methodological and mathematical basis, it is customary to use the following system of transport equations for nonconservative substances [80]:

$$\frac{\partial C_i}{\partial t} + \frac{\partial (uC_i)}{\partial x} + \frac{\partial (vC_i)}{\partial y} + \frac{\partial (w + w_{gi})C_i}{\partial z} - \frac{\partial}{\partial x}\left(D_{xi}\frac{\partial C_i}{\partial x}\right)$$

$$- \frac{\partial}{\partial y}\left(D_{yi}\frac{\partial C_i}{\partial y}\right) - \frac{\partial}{\partial z}\left(D_{zi}\frac{\partial C_i}{\partial z}\right) = F_i(\vec{C}, x, y, z, t) + Q_i(x, y, z, t), \qquad (1.1)$$

where u, v, and w are the components of the vector of current velocity whose three-dimensional field is, in a certain sense, given, $\vec{C}$ is the vector function of the variables of state of the ecosystem $(i = 1, 2, 3, \ldots, N)$ whose elements $C_i(x, y, z, t)$ are the concentrations (biomass) of the modeled components, w_{gi} is the velocity of gravitational sedimentation of the suspended components, D_{xi}, D_{yi}, and D_{zi} are the coefficients of horizontal and vertical turbulent transfer for the i th component, $Q_i(x, y, z, t)$ is the inflow of the i th substance from external sources (including anthropogenic), and $F_i(\vec{C}, x, y, z, t)$ are nonconservative functions constructed on the basis of the balance approach in the form of algebraic sums of terms reflecting the local fluxes of substance between the components of the model caused by various (bio)chemical reactions and biological interactions. Moreover, we have

$$F_i = \frac{\partial C_i}{\partial t} = \left(\frac{dC_i}{dt}\right)_{\text{loc}}.$$

In constructing the numerical model of the quality of water, the three-dimensional space is, as a rule, split into cells (boxes), corresponding to the grid boxes of the hydrodynamic block. It is assumed that, inside a box, the elements of the ecosystem are connected solely by the local fluxes of substance and energy, whereas the transport of substance and energy between the cells is realized as a result of the hydrodynamic transfer.

According to Eq. (1.1), the following blocks are usually selected in the models of water ecosystems:

— the *hydrodynamic block* used to describe the dynamics of waters (currents, the intensity of turbulent transfer, etc.) in the investigated water area under various hydrometeorological conditions with regard for the morphological features of the basin;

— the *block of transfer* of admixtures used to compute the redistribution of admixture over the space in time under the action of currents and diffusion exchange;

— the *block of chemical and biological processes* used to find the nonconservative functions $F_i(\vec{C}, x, y, z, t)$ of modeled substances whose transformations at any local point of the space are realized in the course of chemical, physicochemical, biogeochemical, and/or biological processes.

In the 0-dimensional (point) version of the model of a water ecosystem, the hydrodynamic block and the block of transfer of admixtures are absent and the system of partial differential equations (1.1) degenerates into a system of ordinary differential equations of the form

$$\frac{d\overline{C}_i}{dt} = F_i(\overline{\vec{C}}, t), \tag{1.2}$$

where $\overline{C}_i$ are the values of modeled components of the ecosystem averaged over the bulk of water (or over the basin). Each equation in this system describes the dynamics of the corresponding variable of state of the ecosystem caused by the (bio)chemical reactions and biological interactions between its biotic and abiotic components.

Similarly, we can write the following system of equations used to describe the chemical and biological transformations of substances at a given point of the space:

$$\left.\frac{dC_i}{dt}\right|_{\text{loc}} = \frac{\partial C_i}{\partial t} = F_i(\vec{C}, t). \tag{1.3}$$

In this case, C_i are the local concentrations of modeled elements of the ecosystem averaged over the volume of an elementary cell of the computational grid used in the numerical model.

The nonconservative functions F_i of the system of equations for the biotic and abiotic variables of the model of a water ecosystem are written on the basis of the laws of conservation of substance and energy in the form of balance equations. In the general case, the nonconservative functions for the biotic components of the water ecosystem can be represented in the form

$$F_i = \frac{dB_i}{dt} = P_i - R_i - G_i - M_i, \tag{1.4}$$

where $\frac{dB_i}{dt}$ is the rate of changes in the biomass of the i th biotic variable (component) of the model, P_i is the production created by the i th component per unit time, R_i are its losses for metabolism (respiration) per unit time, M_i is the rate of dying (transition of the living organic matter into the nonliving matter), and G_i is the rate of eating of the analyzed biotic component by the other components.

In the simplest case, each term on the right-hand side of Eq. (1.4) can be represented as the product of the specific rate of the process V_i by the biomass (or biomasses) B_i of the components of the ecosystem participating in this process. The specific rates of the chemical and biological processes are, as a rule, determined empirically. In the simplest case, they are regarded as constant. However, the specific rates of the most significant processes for which the amount of available empirical data is sufficiently large are represented in the multiplicative form as functions of the characteristics of the medium specifying these rates.

1.2. Principal Chemical and Biological Processes Described by the Models of Water Ecosystems

As the main processes studied in the chemical and biological block of models of functioning of the water ecosystems, we can mention

— the process of withdrawal of biogenic elements and primary production of organic substances as a result of photosynthesis;

— the processes of feeding of living organisms (consumers), assimilation of food, and other types of consumption required for vital activities;

— the process of formation of suspended and dissolved inert organic substances as a result of the vital activity and hydrolysis;

— the processes of mineralization of inert organic matter and regeneration of biogenic elements;

— the processes of nitrification and denitrification;

— the processes of mass and gas exchange with bottom sediments and atmosphere.

In what follows, we briefly characterize each of these processes.

In the shelf zones of the sea, the predominant role in the primary production of organic matter is, as a rule, played by phytoplankton. As an exception, we can mention narrow littoral strips and shallow-water sea basins, where the role of macrophytes is comparable with the role of phytoplankton. The process of photosynthesis of the organic matter by algae is determined by their morphological and functional characteristics (volume and specific surface of cells), conditions of illumination, amount of biogenic elements, and the temperature of water.

The illumination of the water column depends on the intensity of flux of photosynthetically active radiation penetrating through the sea surface and the transparency of water. The flux of photosynthetically active radiation is, in turn, determined by the hydrometeorological conditions (cloudiness, humidity, and the state of the water surface) and the transparency of water depends on the concentrations of mineral and organic suspensions (including terrigenous suspension, phytoplankton cells, particles of detritus, etc.).

The amount of biogenic elements available for the algae is determined, first of all, by the concentrations of mineral compounds of nitrogen and phosphorus in water and, for the diatomic algae, in addition, by the concentration of silicon.

Dissolved oxygen is the most important by-product of photosynthesis. The equations used for the description of utilization of biogenic elements and oxygen release in the process of photosynthesis take the form [128]:

$$106\,CO_2 + 16\,NH_4^+ + H_2PO_4^- + 106\,H_2O \rightarrow \text{protoplasm} + 106\,O_2 + 15\,H^+,$$

$$106\,CO_2 + 16\,NO_3^- + H_2PO_4^- + 122\,H_2O + 17\,H^+ \rightarrow \text{protoplasm} + 138\,O_2.$$

The process of nutrition of living organisms (consumers) is described in terms of their rations depending on the morphological and physiological characteristics of organisms of different trophoecological groups (length and weight of the body, its energy equivalent, assimilability of the food, and the efficiency of utilization of assimilated food in the process of growth), selectivity of nutrition, availability of the food, and temperature conditions.

The consumption of substances for the metabolism (respiration) of phytoplankton is evaluated in fractions of the total production of photosynthesis or its current biomass depending on the temperature conditions. The process of respiration is inverse to the process of production. For the living organisms of higher trophic levels (from protozoa to fishes), the consumption of matter for metabolism is evaluated on the basis of empirical relations connecting the rate of metabolism with the weight of the body of animals. The coefficients of these relations are regarded as functions of the temperature of water.

As a result of the consumption for metabolism, the biomass decreases due to the regeneration of biogenic elements accompanied by the utilization of oxygen dissolved in water and direct release of dissolved organic carbon. The relative fractions of these two types of the products of metabolism depend on the amount of oxygen in seawater. In the case where the amount of oxygen is insufficient, the metabolic products in the form of dissolved organic substances are predominant.

Another process decreasing the biomass of living elements of the ecosystem is their mortality, as a result of both natural aging and unfavorable living conditions (including the toxic action of pollutants and/or excrements of the other microorganisms, sharp changes in the temperature or salinity of water, etc.).

The process of formation of inert organic matter includes the process of formation of the products of metabolism, including the nonused remnants food, the process of dying of living population of the water ecosystem (autochthonous organic matter), and the process of transfer of this matter from the other regions (allochthonous matter). The entire inert organic matter is formed by the dissolved (dissolved organic matter) and suspended (detritus; suspended organic matter) fractions. Detritus plays an important trophic role in the water ecosystems. It forms the so-called detrital food chain and is characterized by a nonzero velocity of gravitational sedimentation. As a result of hydrolysis, detritus may pass into the dissolved fraction of the inert organic matter.

With active participation of bacteria, the dissolved fraction of inert organic matter suffers mineralization. We understand mineralization as the process of transition of biogenic elements from the dissolved organic form into the dissolved inorganic form. This process runs under the action of ferments released by bacteria and (possibly) algae [128].

Heterotrophic bacteria use the dissolved organic matter to construct the microbial bodies and satisfy their energy needs. Note that, for bacteria (unlike the other biotic elements of the ecosystem), the coefficient of transformation of the assimilated food into growth varies within the range 0.25–0.33, i.e., more than $2/3$ of the consumed substrate is spent for the vital activities (respiration) of the bacteria [65, 67]. In the course of respiration, the organic matter suffers biochemical oxidation and the biogenic elements are regenerated.

Within the framework of the stoichiometric Richards model, the processes of decomposition, hydrolysis, and oxidation of organic matter under aerobic conditions run according to the following scheme [3]:

$$(CH_2O)_{106}(NH_3)_{16}\,H_3PO_4 \;=\; 106\,CH_2O \;+\; 16\,NH_3 \;+\; H_3PO_4,$$

$$106\,CH_2O \;+\; 106\,O_2 \;=\; 106\,CO_2 \;+\; 106\,H_2O.$$

In the first approximation, it is customary to assume that the intensity of mineralization of the organic compounds of biogenic elements is equal to the intensity of biochemical oxidation of organic matter and that the regeneration fluxes of the mineral compounds of biogenic elements are proportional to their relative contents in the organic matter. Hence, the flux of mineralized organic matter is “split” into elementary components.

The intensity of the process of regeneration of biogenic elements is determined by the temperature of water, the concentration of oxygen in seawater (for biochemical oxidation) and the available biomass of bacteria and, possibly, of phytoplankton since, as follows from [128], the last two characteristics are correlated.

The process of nitrification is initiated by special groups of autotrophic bacteria getting energy for the fixation of carbon dioxide as a result of the oxidation of ammonium to nitrites and nitrites to nitrates. The process of nitrification consists of two reactions (stages) of oxidation, namely,

$$NH_4^+ \;+\; OH^- \;+\; 1.5\,O_2 \;\rightarrow\; H^+ \;+\; NO_2^- \;+\; 2\,H_2O$$

$$\text{and} \qquad NO_2^- \;+\; 0.5\,O_2 \;\rightarrow\; NO_3^-.$$

The intensity of nitrification depends on the temperature of water, its oxygen content, and (indirectly) on the concentration of ammonium.

Under the conditions of insufficient amount of oxygen in seawater, the process of oxidation of organic matter runs due to the presence of oxygen in nitrates (denitrification) [128]:

$$5CH_2O + 4NO_3^- + 4H^+ \rightarrow 2N_2 + 7H_2O + 5CO_2.$$

This process can optionally be initiated by anaerobic heterotrophic microorganisms. Under normal aerobic conditions, these organisms use dissolved oxygen for the oxidation of the organic matter and the process of denitrification runs only for low concentrations or in the absence of dissolved oxygen but in the presence of freely accessible nitrates. The intensity of this process also depends on the temperature of water.

In the shallow-water regions of the sea shelf, the process of functioning of water ecosystems is strongly affected by the mass exchange of biogenic substances with bottom sediments. Detritus and algae cells coming to the bottom sediments as a result of gravitational sedimentation suffer biochemical oxidation and mineralization with participation of the benthos bacteria. These processes may run both under the aerobic and anaerobic conditions.

The decomposition and oxidation of organic matter in bottom sediments can exert a strong influence on the concentrations of biogenic elements and the content of oxygen in the upper layers of the water column. The inorganic compounds of biogenic elements regenerated in the process of biochemical oxidation of organic matter come to the porous waters of bottom sediments and then, as a result of diffusion exchange, to the bottom layer of water. The flux of absorption of dissolved oxygen by the bottom sediments is formed in a similar way. Thus, the bottom sediments can turn into an important source of biogenic elements and a consumer of dissolved oxygen for the adjacent water column. Moreover, in the case of development of anoxia partially caused by the consumption of oxygen by the bottom sediments, the fluxes of some inorganic compounds of biogenic elements (e.g., phosphates [64]) may become much more intense. These elements are liberated from hydroxide compounds with metals (iron, manganese, etc. [64]) as a result of a complex of reactions of reduction.

Dissolved oxygen is required for the existence of higher forms of life in marine media. The concentration of oxygen in seawater determines the distributions of organisms, the rates of the most important biogeochemical redox reactions and, hence, the fluxes of energy and substances in the ecosystem. Therefore, the concentration of dissolved oxygen is one of the most important hydrochemical characteristics of seawater. Furthermore, the process of gaseous exchange with the atmosphere (reaeration) is an important component of the oxygen balance in the water column, especially in the case of deficiency of oxygen. The direction and rate of the process of reaeration are determined by the difference between the actual and saturating concentrations of oxygen which, in turn, depends on the temperature and salinity of seawater. In addition, the rate of reaeration depends on the state of the water surface specified by the wind velocity.

To conclude the general description of the principal chemical and biological processes running in the water ecosystems, we emphasize that their rates strongly depend on the temperature of water. Moreover, as the indicated temperature increases by 10°C, these rates become 2–3 times higher.

1.3. Mathematical Models of the Quality of Waters

The mathematical models of the quality of water can be regarded a special case of the models of functioning of water ecosystems because they are constructed by using similar principles and the main chemical and biological processes specifying the quality of habitat of the hydrobionts and the primary production of organic matter are included in their mathematical structure.

As an important specific feature of these models, one can mention the fact that they are oriented toward the description and prediction of the "fate" of pollutants in water media and their influence on the state of the entire ecosystem evaluated according to the parameters of its trophity, saprobity, and bioproductivity. In these models, the subject of investigations and prediction is, first of all, the quality of habitat of the biotic components of the ecosystem but not the species composition and structure of the trophoecological groups, the trophic links between these groups, and their variability, as in the case of models of functioning of the ecosystems.

Hence, the biotic components in the models of quality of water are, as a rule, maximally aggregated, and the links between them are simplified. Main attention is given to the correct description of the variability of hydrochemical characteristics of the quality of water media and the biotic components of the ecosystem directly connected with the abiotic parameters of the medium by positive and negative feedbacks. Note that the autotrophs and bacteria belong to the indicated class biotic elements of the ecosystem.

According to the character of action upon water ecosystems, all pollutants of chemical nature can be conventionally split into the following two principal groups: eutrophying (biogenic) substances and toxicants. In reasonable concentrations, the biogenic substances are not harmful for the hydrobionts and, moreover, should be regarded as an inherent part of the ecosystem. However, the redundant inflow of these substances in water media may lead to negative effects in the process of functioning of the ecosystems.

Under natural conditions, the biotic turnover of substances in marine ecosystems is balanced and, hence, the entire water-medium–biota system is in the state of phase equilibrium in biogenic substances, i.e., the intensity of the process of primary production of the organic matter by phytoplankton accompanied by the consumption of mineral compounds of nitrogen and phosphorus is, as a final result, compensated by the rate of their regeneration in the process of biochemical oxidation of metabolic excretions and dead fragments of hydrobionts (inert organic matter) by heterotrophic bacteria. The uncontrolled penetration of large amounts of biogenic substances of the anthropogenic origin in marine media leads to the increase in the rate of primary production of the organic matter, which cannot be assimilated by the organisms of higher trophic levels and, hence, its dying creates favorable conditions for the development of heterotrophic bacteria. As a result, the period of turnover of biogenic substances in the ecosystem sharply decreases and the consumption of oxygen for the biochemical oxidation of organic matter (with participation of bacteria) increases.

The process of increase in the level of trophity of a water area (basin), i.e., in the level of formation of new organic matter in the process of biological production is called eutrophication. On the level of ecosystems, this process has the following consequences:

— changes in the chemical conditions formed in the analyzed water area;

— formation of the deficiency in oxygen (hypoxia) or its complete disappearance in the bottom layers of water (anaerobiosis of marine media);

— sharp deterioration of the living conditions for higher hydrobionts;

— violation of balance between the processes of production and destruction, stability, trophic structure, and the dynamics of functioning of the ecosystem.

Note that, in closed basins, the development of the process of eutrophication can be explained by natural causes, e.g., by shallowing of the basin [23].

The water ecosystems contain, in fact, a significant internal source of mineral compounds of biogenic elements, i.e., their regeneration in the course of biochemical oxidation of organic matter. Therefore, for the adequate description of the negative effects of eutrophication in the model, it is necessary to consider the balance of production and destruction processes in the ecosystem, i.e., the closed biogeochemical cycles of the principal biogenic elements responsible for the primary production of organic matter in the analyzed parts of water area of the sea (or other basins).

The models of the quality of water taking into account the effects of eutrophication include, as a rule, the biotic components of the ecosystem and their structure is compatible with the structure of the models of functioning of water ecosystems. In fact, they represent the lower hierarchical level of the models of ecosystems with maximum possible aggregation of the biotic components. As for the level of organization (complexity) of the chemical and biological block, these models belong to the class of self-adapting models whose parameters change with the state of the system but the structure remains unchanged [92].

Unlike biogenic elements, the pollutants of toxic action are themselves harmful for the hydrobionts because they suppress the development of hydrobionts, increase their mortality, and decrease the birth rate. As a result of action of these pollutants, the processes of functioning of the ecosystem as a whole and some of its biotic components as well as the balance of the processes of production and destruction are violated, the trophic structure of the ecosystem changes, and the recreational and biological resources of the marine medium decrease.

In most cases, toxic pollutants are of the anthropogenic origin. Thus, in the absence of anthropogenic influence, they are never detected in the concentrations harmful for hydrobionts. The substances from this class have no significant natural sources inside the ecosystems. Hence, in the case of appearance of these substances in marine media, their concentration permanently decreases both with time and with the distance from the source of pollution as a result of the combined action of the processes of self-cleaning, including the hydrodynamic dilution, various microbiological and biological transformations, chemical and physical transformations, sedimentation of the mineral particles of suspension, and biosedimentation.

As typical examples of pollutants from this class, we can mention, e.g., the synthetic surfactants, oil products, phenols, and heavy metals.

The dynamics of pathogenic bacteria in water media is similar to the dynamics described above and the decrease in their quantity is explained by the mortality of microorganisms under the conditions unfavorable for their development.

For the description of the dynamics of this type of pollutants in marine media, the chemical-and-biological block of models of the quality of water is usually constructed as a block of self-cleaning of waters, i.e., the feedbacks between the components of the model are neglected and only the decrease in the concentration of pollutants as a result of the combined action of physical, chemical, and biological processes is described. In the applied models of the quality of water, the role of separate chemical and biological processes promoting the self-cleaning of waters is often not specified explicitly and described in the form of parametric dependences between the total rate of destruction of pollutants and the physicochemical characteristics of water media affecting this process (temperature, salinity, pH value, etc.). As a rule, the transition of pollutants through the trophic chains and the secondary effects of pollution are neglected in the models of self-cleaning.

In view of the indicated separation of pollutants into two main groups (eutrophying and toxic), the chemical-and-biological block of the model of quality of waters includes, in the general case, the (sub)blocks aimed at the solution of the following problems:

— self-cleaning of waters from pollutants untypical of the marine medium, i.e., coming into the ecosystem from the external (as a rule, anthropogenic) sources;

— eutrophication and the oxygen conditions of waters used to describe the natural chemical and biological processes specifying the balance of substances and energy in the ecosystem and the degree of trophity and saprobity of its waters.

The mathematical structure of these blocks is described in detail in the subsequent chapters of the present monograph.

The application of mathematical models for the solution of the applied problems of the ecology of sea is based on the use of certain quantitative criteria for the evaluation of the state of the ecosystem and the quality of its waters. For the toxic pollutants, the role of a criterion of this sort is payed by their maximum permissible concentrations determined by the type of water consumption [3, 78, 89]. However, for biogenic elements, the existing maximum permissible concentrations do not reflect their actual role in the process of functioning of marine ecosystems and, hence, cannot be used in the solution of applied problems dealing with the analysis of development of the process of eutrophication.

The application of common standard criteria of maximum permissible concentrations for the control over the quality of seawater should be regarded solely as the first approximation. Indeed, these criteria form necessary but not sufficient conditions for guaranteeing the ecological safety of the shelf zone of the sea. For the complex solution of this problem, it is necessary to use the second group of criteria, namely, the ecological standards of the quality of water characterizing the composition and properties of water as an essential constitutive part of the water ecosystem and the habitat of hydrobionts [62, 112, 113, 115].

Unlike the surface waters of inland basins, there are no common criteria for the evaluation of the ecological state of marine ecosystems. Hence, the degrees of trophity and saprobity of the shelf seawater are, as a rule, estimated according to the traditional criteria: the concentrations of mineral compounds of nitrogen and phosphorus, the oxygen equivalent of concentration of the labile part of the inert organic matter [BOD (biochemical oxygen demand), BOD_5, and permanganate oxidizability], and the concentration of oxygen in the bottom layer. The values of these parameters for the coastal parts of the sea and the estuaries of rivers subjected to the anthropogenic load are compared with the background levels typical of the open part of the sea. In this case, the concentration of inert (nonliving) organic matter is regarded as an indirect characteristic of the saprobity of waters and the concentrations of oxygen and mineral compounds of nitrogen and phosphorus serve as a characteristic of the trophity of waters in the analyzed region.

In our opinion, the concentration of mineral compounds of nitrogen and phosphorus (which does not affect the rate of photosynthesis) can serve as an ecological criterion of the quality of seawater as far as presence of these compounds is concerned. The analysis of the available literature sources shows (Subsection 5.1) that, for the major part of littoral marine ecosystems suffering eutrophication, the maximum concentrations of mineral compounds of nitrogen and phosphorus for which they still limit the primary production of phytoplankton are equal to $0.1\ \text{mgN/liter}$ and $0.02\ \text{mgP/liter}$, respectively. Thus, if the indicated concentrations are exceeded in the photic layer in the period of vegetation, then this means that, as a result of eutrophication, the process of production of phytoplankton is no longer controlled by the concentrations of biogenic elements in seawater.

1.4. Brief Survey of the Models of Functioning of Water Ecosystems and the Formation of Quality of Their Waters

The appearance of the first complex models of marine ecosystems is connected with the rapid progress in the development of computers in the middle of the 1980s. Note that a significant contribution to the development of the theory of mathematical models of marine ecosystems was made by Soviet researchers. Thus, the theoretical foundations, basic principles of construction, and procedures of numerical realization of mathematical models of the behavior of marine biogeocenoses were formulated for the first time in the monograph [66]. On the basis of the analysis of incomplete literature data, the authors collected the information required for the mathematical description of the principal processes of mass exchange in marine ecosystems, deduced the corresponding computational formulas, and got the required numbers. It is worth noting that various principles proposed in [66] for the description and parametrization of the ecosystem processes remain actual up to now.

In the monograph [80], the ideas presented in [66] were developed and partially realized in the form of the specific results of numerical simulations of the Baltic-Sea ecosystem. In the cited book, one can also find the results of modeling of both the many-year dynamics of biogenic substances in the sea (in the 0-dimensional space version) and the evolution of the vertical structure of the turnover of substances in the sea (nonstationary model of ecosystem with resolution in depth). In addition, a submodel of interaction of the pelagic part of the marine ecosystem with its benthic part was constructed. Note that the hydrodynamic and chemical-and-biological parts of the problem of modeling of marine systems were studied separately and solved almost independently.

The problem of modeling of the horizontal variability of hydrochemical and biological components of the shelf ecosystem of the northwest part of the Black Sea depending on the anthropogenic factors and hydrological conditions was studied in [5]. Although the hydrodynamic and chemical-and-biological parts of the problem were solved separately, the discrete current fields obtained within the framework of the hydrothermodynamic model were used for the description of mass exchange between different points of the investigated region. The chemical-and-biological block of the model includes seven components: phytoplankton, macrophyte algae, zooplankton, fishes, mineral nitrogen and phosphorus, and inert organic matter. In the cited work, the methodical aspects of application of the mathematical models of marine ecosystems to the solution of the practical problems of rational utilization and preservation of the resources of the shelf zone of the sea found their subsequent development.

A model of functioning of spatially inhomogeneous phytocenoses in the littoral parts of the sea subjected to anthropogenic loads was proposed in [18]. This model consists of three blocks: a three-dimensional diagnostic hydrodynamic model for the analysis of wind currents, a two-layer block of transfer of admixtures in the horizontal plane, and a chemical-and-biological block including the following variables: seven size groups of phytoplankton, labile fraction of detritus, mineral nitrogen and phosphorus, and dissolved oxygen. As a specific feature of this model, we can mention the fact that the rates of chemical and biological processes are described by complex nonlinear functions of the factors affecting these processes. The coefficients of these functional dependences were determined experimentally under the laboratory conditions. This fact seems to be the main disadvantage of the model because the procedure of calibration of its parameters is quite complicated and the universal character of these parameters is doubtful. For this reason, the authors proposed to use this model for short-term predictions of the ecological state of littoral waters in the northwest part of the Black Sea.

A substantial progress in the field of mathematical description of functioning of marine ecosystems was connected with the appearance of a mathematical model developed under the guidance of Academician M. E. Vinogradov at the Institute of Oceanology of the Academy of Sciences of the USSR [15, 65, 168]. This model is characterized by the presence of a universal theoretically and methodologically substantiated scheme of finding the fluxes of substance and energy between the biotic elements of pelagic ecosystems.

The indicated scheme is based on the data of *in-situ* simultaneous complex evaluation of the biomasses of the main biotic elements of the marine ecosystem and the average mass of a single object of each element. If these quantities are known, then, by using the computational scheme, one can find the production, respiration, the total and partial rations, and the rate of eating of each element of the plankton community. The structure of the model imposes almost no restrictions on the number of modeled biotic elements of the marine ecosystem. The model was used for the description of functioning of the plankton communities in the Black Sea and in the tropical regions of the Pacific Ocean. Thus, the seasonal course of the biomasses of elements of the ecosystem and their vertical and horizontal space structures were modeled in [65]. Moreover, an original procedure of combining the results of the hydrodynamic and chemical-and-biological blocks of a large-scale model of pelagic ecosystem was used for the Black Sea.

Although the model proposed at the Institute of Water Problems of the Academy of Sciences of the USSR [49, 50] was developed for closed inland basins, it also is of interest for our purposes because the structure of its chemical-and-biological block most completely meets the requirements imposed on the applied models of the quality of water for marine ecosystems. This model is characterized by the explicit mathematical description of the role of bacterial plankton in the biochemical oxidation of the inert organic matter and regeneration of the mineral compounds of nitrogen and phosphorus. The model includes four biotic elements of the ecosystem (phytoplankton, bacteria, protozoa, and zooplankton) and nine abiotic elements (dissolved and suspended organic nitrogen and phosphorus, ammonium, nitrite, and nitrate nitrogen, dissolved mineral phosphorus, and oxygen). The structure of the model makes it possible to describe the entire complex of interacting physical, chemical, and biological processes connected with the transformations of organic substances and nitrogen and phosphorus compounds and the biochemical consumption of oxygen. This model was initially developed and calibrated (according to the data of experiments in microcosms) for marine media [1, 2] but found its practical application for closed freshwater basins [50]. Therefore, this model is used without hydrodynamic block in the local (0-dimensional) space version [48, 50].

Parallel with the already mentioned models, various versions of the models of functioning of water ecosystems can also be found in [4, 41, 44]. These models are of interest from the viewpoint of the procedures of their calibration and verification, evaluation of their sensitivity, and the specific features of parametric description of the rates of various chemical and biological processes.

An attempt to give an explicit description of the role of bacteria in modeling the turnover of nitrogen and phosphorus in freshwater ecosystems was made in [31, 32]. However, these models are too formalized and contain a great number of difficultly determined coefficients. Hence, they can hardly be used in practice for the solution of the applied problems of control over the quality of water resources.

In [67], one can find an original version of the model of self-cleaning of waters in the shelf zone of the sea from organic matter and mineral forms of biogenic substances penetrating as a part of industrial and municipal sewage waters from the local sources of pollution. This model can be used, as the first approximation, for the evaluation of the dimensions of the zone of pollution and permissible volumes of discharge of the industrial and municipal sewage waters through sea waste pipes and the analysis of the influence of river discharge on the neighboring water area of the sea.

As far as the foreign models are concerned, the following applied models of the quality of waters are highly renowned by the world scientific community and find extensive practical applications in numerous countries: MIKE-21-WQ of the Danish Hydraulic Institute [129], WASP5 (Water Quality Analysis Simulation Program) of the US Environmental Protection Agency [118], and the CE-QUAL-ICM three-dimensional model of eutrophication of the US Army Corps of Engineers [128]. These models were developed for the solution of applied problems of preservation of marine media and used, as a basis, for the creation of the well-known software products aimed at the analysis of the quality of water (ECOM/POM, WASP/RCA, and HydroQual/Delft3D). They are extensively used in different countries for the ecological expert analyses of various engineering projects connected with the utilization and preservation of water resources.

In the version of the MIKE-21-WQ model available for the authors, the biomass of phytoplankton is not a variable of the model. The model takes into account the utilization of biogenic substances by phytoplankton in the process of photosynthesis by specifying its production regarded as constant and independent of the external factors. Hence, the regeneration of the mineral forms of biogenic substances in the course of biochemical oxidation of inert organic matter is not taken into account, i.e., the indicated model belongs to the class of models of self-cleaning but used for the description of the process of eutrophication.

The American WASP5 and CE-QUAL-ICM models have more complex mathematical structures. Thus, the WASP5 model has two blocks: the block of modeling of the quality of water under the action of toxic pollutants and the block of modeling of the process of eutrophication. The eutrophication block has eight variables specifying the processes of production and destruction of the organic matter, utilization and regeneration of the mineral forms of biogenic substances in the ecosystem, and the oxygen conditions of the basin, namely, the nitrogen of ammonium and nitrates, inorganic phosphorus, phytoplankton, biochemical consumption of oxygen, dissolved oxygen, and organic nitrogen and phosphorus. The phosphorus and nitrogen cycles are described in the model separately and combined on the basis of the equation of dynamics of phytoplankton. The process of eating of phytoplankton by zooplankton is explicitly described by specifying the annual course of the biomass of zooplankton in waters of the investigated region established according to the data of observations. The mass exchange between water and bottom sediments is evaluated.

The CE-QUAL-ICM eutrophication model was developed for the Chesapeake Bay. The principles of construction of the mathematical structure of this model agree with the WASP5 model but the analyzed model is more complex and systemic (in the description of feedbacks between the modeled elements of the ecosystem). The principal variables of this model include three groups of phytoplankton, nitrogen of ammonium and nitrates, phosphates, organic nitrogen, phosphorus and carbon (split into the dissolved, suspended labile, and stable fractions), chemical consumption of oxygen, dissolved oxygen, dissolved silicon, and suspended biogenic silicon. The model includes a block for the evaluation of mass exchange with bottom sediments in the diagnostic and prognostic modes.

It should be emphasized that the principles used for the construction of the CE-QUAL-ICM model completely correspond to the domestic theoretical results described in the monograph [66] published much earlier.

In the major part of the models developed abroad, the role of bacteria in the formation of the quality of waters is parametrized by specifying the coefficients characterizing the rates of the corresponding biogeochemical processes. As an exception from this rule, we can mention the classical biogeochemical model of the dynamics of plankton [134] based on the nitrogen cycle. This model includes the following seven variables: phytoplankton, zooplankton, bacteria, nitrogen of ammonium and nitrates, labile dissolved organic nitrogen, and detrital nitrogen. Later [155], this model was combined with the hydrodynamic model of large-scale oceanic circulation and, in its three-dimensional version, applied to the investigation of the seasonal variability of the fields of chemical and biological characteristics of waters in the North Atlantic. This model was also used as a chemical-and-biological block of the three-dimensional ecological model of the Black Sea for the reconstruction of the seasonal variability of the components of its ecosystem [39].

As follows from the survey presented above, the main attention of the domestic researchers was given to the development of comprehensive mathematical models of functioning of water systems with complex mathematical structure depending on the large number of empirically determined coefficients. The application of these models to the solution of applied problems, i.e., in planning the consumption of water for various objects is quite difficult because requires the use of significant amounts of the resources to equip these models with the initial chemical-and-biological data, for calibration of the parameters, and verification. Moreover, the methodological aspects of the evaluation of numerous parameters of these models and the coefficients of the corresponding functional dependences are developed quite poorly, which naturally leads to the ambiguity of the results and recommendations obtained by using these models.

At the same time, the applied models of the quality of water developed by foreign (American and European) researchers combine both the comprehensiveness and adequacy of the description of natural processes specifying the quality of water media and informativeness of the results of modeling with the minimization of the resources used to prepare the initial data for the operation of the model, its adaptation (calibration), and verification. In these models, the role of variables of state for water ecosystems is played by the standard hydrochemical characteristics of the quality of seawater and the minimum amount of hydrobiological parameters. The indicated properties enable us to use these models for the solution of a broad range of applied problems of the ecology of sea.

Conclusions

The systematic increase in the anthropogenic load acting upon the ecosystems of the sea shelf leads to a substantial deterioration of the quality of water media, violation of the natural balance of biogeochemical processes, and changes in the productivity, structure, and regularities of functioning of the ecosystems. As a result, the biological resources of marine media are deteriorated and their recreational potential decreases. In this connection, the problem of control over the quality of marine media by means of the realization of various projects of preservation of nature aimed the reduction of the anthropogenic load upon the littoral marine ecosystems and enhancement of their self-cleaning potential seems to be quite urgent. Mathematical modeling proves to be the main method of ecological planning, prediction, and estimation of correctness and adequacy of various administrative decisions in the fields of management of the marine resources and preservation of nature.

The mathematical models of water ecosystems based on the principles of systems analysis enable one to make decisions with regard for the correlations between the components of the ecosystem and transform ecological predictions from the category of intuitive into objective. They play the role of a link between the ecological theory, scientific investigations, and practical control over the quality of water media.

The mathematical models of the quality of water represent a special case of the models of functioning of water ecosystems in which principal attention is given to the description of the evolution of pollutants and the variability of the abiotic characteristics of the ecosystem specifying the quality of water media for the life of hydrobionts and utilization by the society.

According to the character of their action upon water ecosystems, all pollutants of chemical nature are split into the following two main groups: eutrophying (biogenic) substances and toxicants. The dynamics of these groups of pollutants is described by the models of the quality of waters in different ways. Thus, in the first case, it is customary to use simplified modifications of the models of functioning of water ecosystems in which the biotic components are aggregated to the maximum possible extent. In the second case, it is necessary to solve the problem of self-cleaning of waters in which the feedbacks between the components of the model are neglected and the concentration of pollutants decreases as a result of the combined action of physical, chemical, and biological processes.

The complex multipurpose spatially resolving models of the quality of seawater include a numerical hydrodynamic model, a block of transfer of admixtures, and a chemical-and-biological block [which, in turn, consists of the (sub)blocks of eutrophication and self-cleaning of waters from pollutants].

As quantitative criteria for evaluation of the efficiency of various administrative decisions aimed at the preservation and improvement of the quality of littoral seawater, one can use the values of maximum permissible concentrations for the toxic pollutants and the degree of approach of the predicted concentrations in the littoral parts of the sea subjected to anthropogenic loads to the background values typical of the open part of the water area for the eutrophying pollutants. For the mineral forms of biogenic substances, it is proposed to use their ultimate concentrations corresponding of threshold of limitation of the primary production of phytoplankton by each of these substances in the vegetation period as the ecological standards of the quality of waters.

The analysis of the domestic and foreign mathematical models of the quality of waters in marine ecosystems and the application of these models to the solution of various problems of the ecology of sea shows that the problem development of domestic complex mathematical models of the quality of seawater satisfying all contemporary requirements, which can be used for the solution of a broad range of applied problems of management of the marine resources and preservation of nature, is quite urgent. Actually, the problem is not only to propose the mathematical structure of the model and its software realization but also to develop the procedures of calibration of its parameters, including the accumulation of all necessary primary data, and the procedures of using of the model with an aim to get practically significant results.

2. PHYSICOGEOGRAPHICAL AND ECOLOGICAL DESCRIPTION OF THE ANALYZED MARINE WATER AREAS

The methodology of development of numerical mathematical models aimed at the solution of applied problems of preservation, restoration, and rational utilization of the sea-shelf resources is developed and tested for two regions of the World Ocean with different climatic conditions: the northwest part of the Black Sea and the Colombian part of the shelf zone of the Caribbean Sea.

The tropical marine ecosystems are of significant interest as subjects of mathematical modeling because, due to the negligibly weak seasonal variability of temperature conditions, they could be regarded as a perfect object of testing of the mathematical structure of the chemical-and-biological blocks of the models for the adequacy of the description of the actual links between the inert and biotic components of the ecosystem and the factors affecting these links.

Unlike the tropical ecosystems, the water ecosystems of middle latitudes are characterized by the well-pronounced seasonal variability of the hydrological, chemical, and biological characteristics caused by the predominant influence of the annual course of the temperature of water on the rates of chemical and biological processes specifying the fluxes of substance and energy between the components of the ecosystem.

In modeling the quality of waters in the marine ecosystems of middle latitudes, the role played by the thermohydrodynamic block becomes more pronounced because, in this case, the model must give an adequate description of the processes of formation of the vertical thermohaline structure of waters and the annual course of the temperature of water in the modeled water area at different depths. The procedure of calibration of the parameters of the chemical-and-biological block of the model becomes quite complicated because the predominant influence of the variations of the temperature of water makes it difficult to detect the specific features of interactions between the components of the model caused by the other factors.

The main subject of ecological investigations and modeling at middle latitudes studied in the present work is the Odessa region of the Dnieper–Bug estuary zone in the northwest part of the Black Sea (Fig. 2.1). The quality of waters in this region of the Black Sea is formed under the influence of the river discharge of the Dnieper and Yuzhnyi Bug and the anthropogenic sources of pollution located in the coastal zone of the Odessa region.

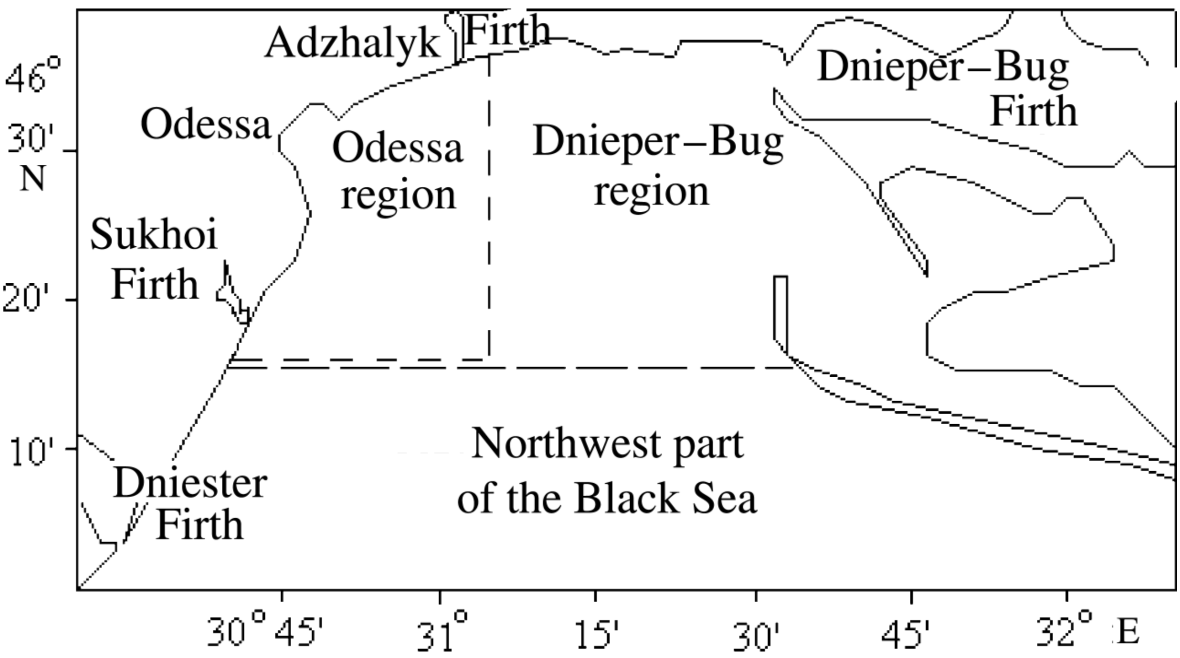


Fig. 2.1. Geographical position of the Dnieper–Bug and Odessa regions in the northwest part of the Black Sea.

The possibilities of application of the hydrodynamic block to the solution of applied problems of management of the marine resources are demonstrated by analyzing an example of the Tuzla group of firths located in the interfluve of the Danube and Dniester.

On the Colombian shelf of the Caribbean Sea, we study three coastal basins partially isolated from the neighboring water area of the sea: the Cartagena Bay, the shallow-water Ciénaga-de-Tesca Lagoon, and the shallow-water Ciénaga-Grande-de-Santa-Marta Firth (Fig. 2.2). The Cartagena Bay and the Ciénaga-Grande-de-Santa-Marta Lagoon were artificially transformed into estuary-type marine basins. Note that the ecosystems and the quality of waters in these three basins suffer strong anthropogenic actions and require reconstruction.

The Colombian shelf of the Caribbean Sea belongs to the tropical zone of the World Ocean [45]. The waters of this region are characterized by high levels of salinity (≈ 35‰) and temperature (29–33°C). The vertical stratification of waters and the seasonal variability of the hydrological characteristics are weakly pronounced. The amplitudes of seasonal and short-period variations of the temperature of water are comparable.

The Colombian coast is characterized by the presence of tidal oscillations of the sea level. They can be classified as mixed irregular daily tides 20–40 cm in height.

In what follows, on the basis of the data of ecological monitoring, we describe the established (by the authors) specific features of the formation of the quality of waters in the investigated shelf zones of the sea, their hydrological and hydrochemical conditions, and primary productivity and formulate the ecological problems whose solution requires the development of adequate mathematical models.

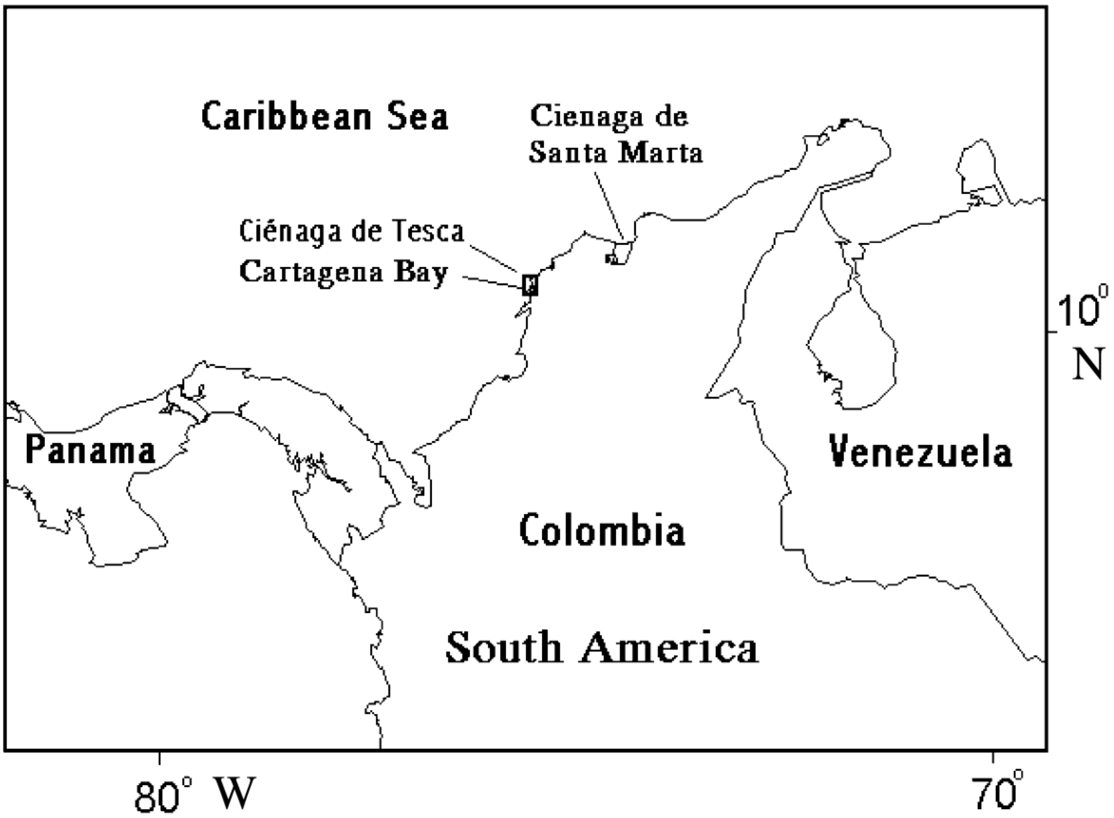


Fig. 2.2. Geographical position of the investigated basins of the sea in the Colombian part of the shelf zone of the Caribbean Sea.

2.1. Tropical Sea Basins of the Colombian Coast of the Caribbean Sea

This region is characterized by the dry tropical climate. Every year has four typical seasons: dry season (December–April), short rainy (May–June) and short dry (July–August) seasons (often combined under a single name of transient season), and rainy season (also called wet; September–November). In the dry season, the north and northeast trade winds are predominant and, during a day, their velocity varies from 1 m/sec in the morning to 10–15 m/sec during the daytime and in the evening. In May, as the transient season begins, the winds become weaker and do not have any predominant direction. The rainy season is characterized by the presence weak south equatorial winds.

The interannual variability of the quality of waters and productivity of the ecosystems of sea basins in the Colombian part of the shelf of the Caribbean Sea has cyclic nature explained by the climatic factors connected with the development of events of El Niño in the Pacific Ocean. The years characterized by the presence of El Niño are low cloudy and low water due to the small amounts of atmospheric precipitation. The rainy season is fairly short and weakly pronounced. Then the year of El Niño is replaced by the period of La Niña and the next year, on the contrary, is high water with large amounts of atmospheric precipitation.

The amount of water in a year strongly affects the ecological state of the estuarine ecosystems because the larger the amount of atmospheric precipitation, the larger the amount of pollutants washed away from the water-catchment area and, hence, the higher the flow rate and the level of pollution of river waters. On the other hand, the periods of intense precipitation are characterized by high levels of cloudiness. Therefore, the flux of photosynthetically active radiation coming to the water surface decreases. The increase in the river discharge leads to the increase in the amount of suspension coming with it to the sea and, hence, the transparency of seawater becomes lower and the depth of the photic layer decreases.

2.1.1. Sea Tropical Deep-Water Cartagena Bay

The Cartagena Bay is located on the Colombian coast of the Caribbean Sea in a square bounded between $10°16'-10°26'$ N and $75°30'-75°35'$ W (Fig. 2.3). The bay has the following morphological characteristics: its maximum lengths in the meridional and latitudinal directions are ≈ 16 and 9 km, respectively, the area of water surface is ≈ 82 km^2, its mean depth is equal to 16 m and its maximum depth to 26 m (Fig.A.1). The bay consists of two parts: the Outer Bay connected with the Caribbean Sea by two straits and the Inner Bay located to the north and connected with the sea only via the Outer Bay. The historically well-known city-port of Cartagena is located on the coasts of the Inner Bay and 40% of its raw municipal sewage waters are discharged into the bay. Moreover, 29 industrial enterprises are located in the industrial zone of Cartagena on the east coast of the Outer Bay. The total flow rate of the anthropogenic sources is $\approx 1.42 \cdot 10^6$ m^3/day. Every day these sources deliver into the bay waters ≈ 2.57 tons of mineral nitrogen compounds, 0.48 tons of mineral phosphorus, and 22.2 tons of inert organic matter (by the BOD). The location of these sources and the characteristics of their waters are presented in Fig. 2.3 and Tables B.1 and B.2.

Fresh waters penetrate into the south part of the Outer Bay through the Dique Channel connecting the bay with the River Magdalena. This channel was made artificially. During a year, its flow rate varies from 55 m^3/sec in the dry season (February–April) to 250 m^3/sec in the rainy season (September–October).

The Dique Channel affects the hydrochemical conditions in the bay in two ways. On the one hand, the channel is a powerful supplier of mineral compounds of nitrogen and phosphorus and mineral suspension specifying the transparency of waters in the bay. On the other hand, a sharp subsurface (0–4 m) pycnocline inhibiting the vertical turbulent exchange between the surface and bottom layers is formed in the bay under the influence of the freshwater discharge of the channel. As a result, the biogenic substances and other pollutants carried out by the waters of the channel are distributed over the water area of the bay inside the surface freshened layer, which also plays the role of the photic layer.

As a result of the penetration of large amounts of mineral suspension into the bay with waters of the Dique Channel and its subsequent gravitational sedimentation, we observe the process of shallowing of the wharves located on the coasts of the bay and the intense accumulation of sediments in the artificial navigation channel in the south part of the bay.

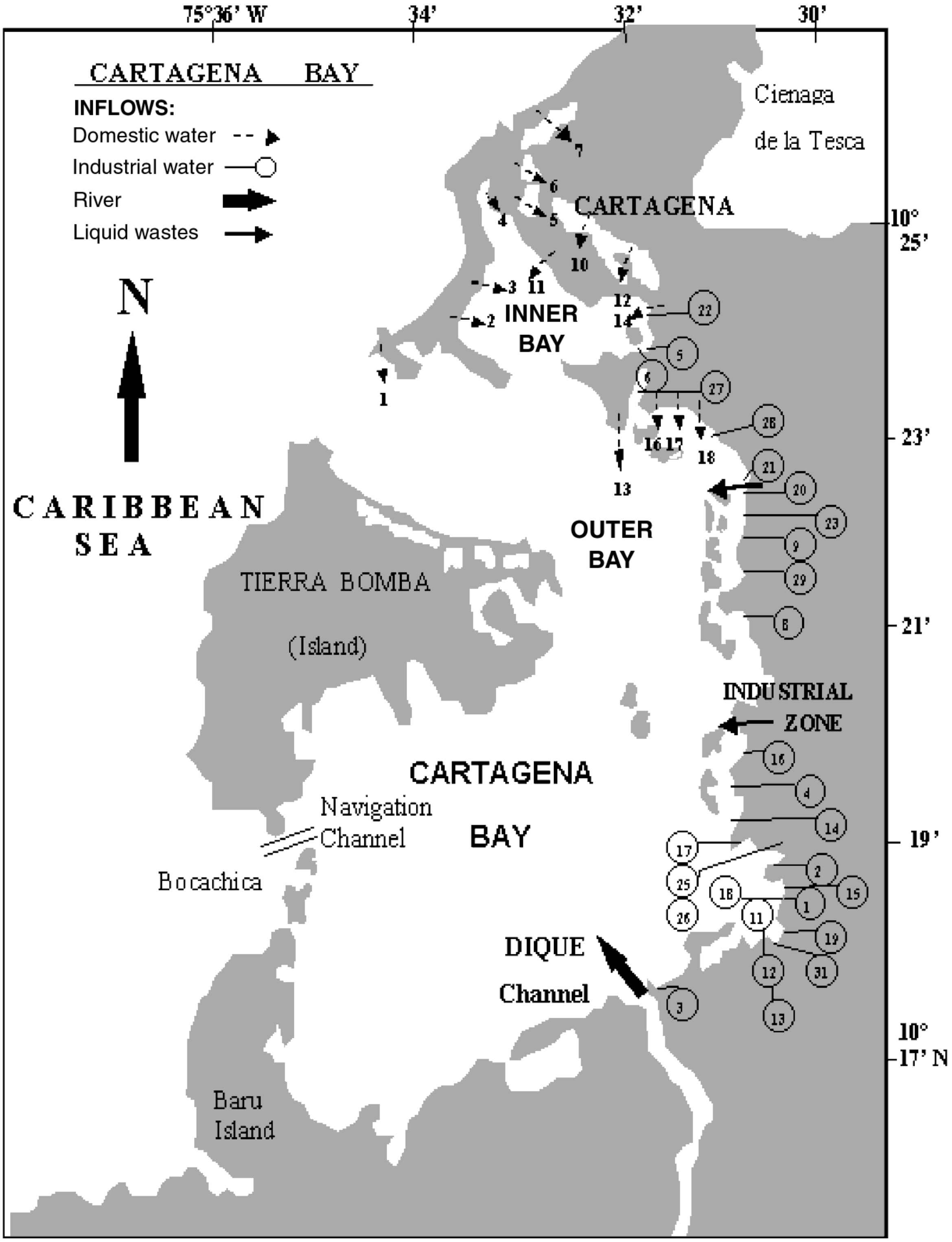


Fig. 2.3. Schematic diagram of the Cartagena Bay with the anthropogenic sources of pollution.

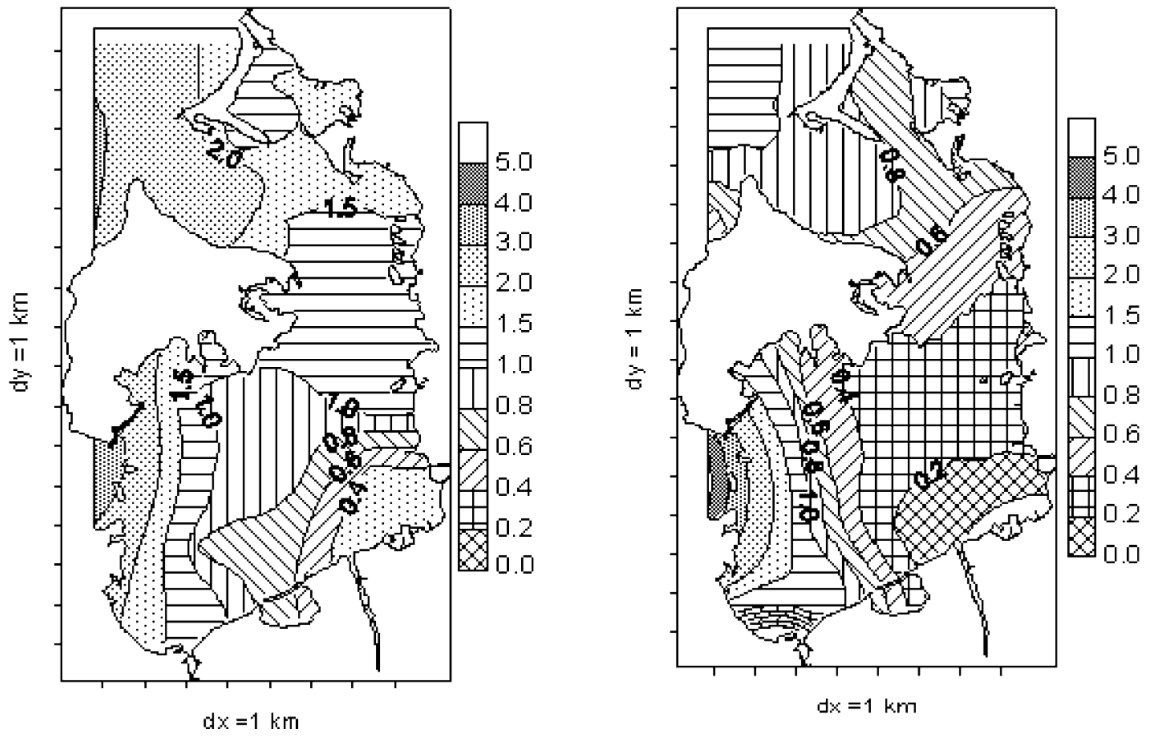
Thus, near the wharves of industrial enterprises located in the south part of the bay, the depth of the sea decreased by 5–6 m for the last 15 yr and, hence, many of these enterprises are forced to perform annual dredging works.

The ecological monitoring of waters in the Cartagena Bay was carried out by the Colombian Centro Investigaciones Oceanográphicas e Hydrográphicas (CIOH) in 1996–1999 [143, 152, 153]. The program of monitoring included 2–5 annual surveys with up to 23 stations in the water area of the bay. The following parameters were measured: the transparency, temperature, and salinity of water, the concentrations of mineral compounds of biogenic elements and dissolved oxygen, the biochemical oxygen demand, and the concentrations of chlorophyll A at depths of 0.5 and 8 m and near the bottom. In addition, the program included one-time hydrobiological measurements of the primary production of phytoplankton, the biomass of bacterial plankton, and the flux of absorption of oxygen by the bottom sediments. The level of pollution of waters in the bay with pathogenic bacteria was systematically monitored by analyzing their indicator, i.e., the total number of Coliform bacteria (an analog of the coli-index) [165].

In Table 2.1, we present the concentrations of biogenic elements and biochemical oxygen demand typical of the photic layer in waters of the Dique Channel, Cartagena Bay, and at the open sea boundary of the bay obtained as a result of averaging of the data of ecological monitoring for 1996–1998. As follows from Table 2.1, the concentrations of mineral compounds of biogenic elements in waters of the bay are quite high and, hence, do not play the role of a factor limiting the rates of primary production of the organic matter by phytoplankton. In this case, the role of a factor suppressing the process of photosynthesis of phytoplankton is played by the mineral suspension coming to the bay with waters of the channel. The indicated suspension substantially decreases the transparency of seawater and the depth of the photic layer and, therefore, strengthens the role of the hydrodynamic processes of dilution of the polluted waters of the bay with pure waters of the sea. The typical fields of transparency of waters in the bay for the dry and wet seasons of a year are presented in Fig. 2.4.

Table 2.1. Hydrochemical Parameters of the Quality of Waters in the Dique Channel, Photic Layer of the Cartagena Bay, and at the Open Boundary of the Bay with the Caribbean Sea

Hydrochemical parameter	Dique Channel	Cartagena Bay	Sea boundary
BOD_5, mg O_2/liter	1.31	2.1	0.7
NH_4^+, mgN/liter	0.14	0.12	0.05
NO_2^-, mgN/liter	0.004	0.006	0.002
NO_3^-, mgN/liter	0.25	0.065	0.007
PO_4^{3-}, mgP/liter	0.04	0.023	0.018
O_2, mg O_2/liter	4.0	5.0	4.25

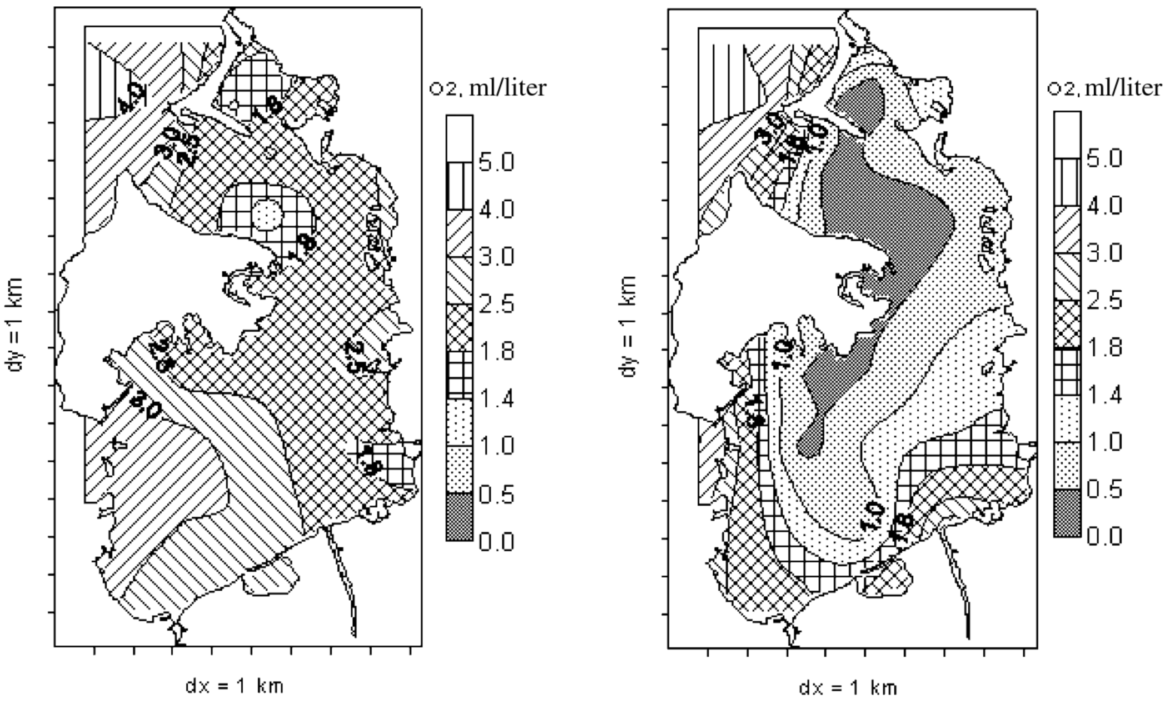


(a) **(b)**

Fig. 2.4. Typical fields of the transparency of waters in the Cartagena Bay (in meters) for the dry (a) and wet (b) seasons of a year plotted according the data of monitoring for 1996–1999.

Moreover, the process of intense sedimentation increases the mortality of benthic organisms and impedes the development of zooplankton in the bay. Toxic substances adsorbed by suspended particles can be dangerous both for the life of hydrobionts and for the health of the people. This is why the Colombian institutions interested in the solution of the problems of pollution developed various projects of construction of hydraulic structures in the Dique Channel aimed at the reduction of the inflow of suspended substances from the channel into the Cartagena Bay. Clearly, these projects should be subjected to the ecological expert examination from the viewpoint of possible consequences of their realization for the process of functioning of the ecosystem of the Cartagena Bay and the quality of its waters.

The depth of the straits connecting the bay with the sea, as a rule, equal to 0.5–3.0 m. However, this is not true for the navigation channel in the south strait 100 m in width whose depth is equal to 30 m. Since the maximum depths in the Cartagena Bay can reach 26 m, the process of hydrodynamic washing of the bottom layers of the bay by waters from the sea is obstructed. The tidal oscillations of the sea level on the open sea boundary promote the renewal of waters in the bay as a result of the horizontal advection of pure seawater. It is worth noting that the density of water in the open sea is higher (due to its higher salinity) than the density of freshened waters in the bay. Therefore, on passing through the shallow straits, the waters coming from the sea flow down into the deeper layers of the bay toward the bottom, thus renewing the waters of the bottom layer.



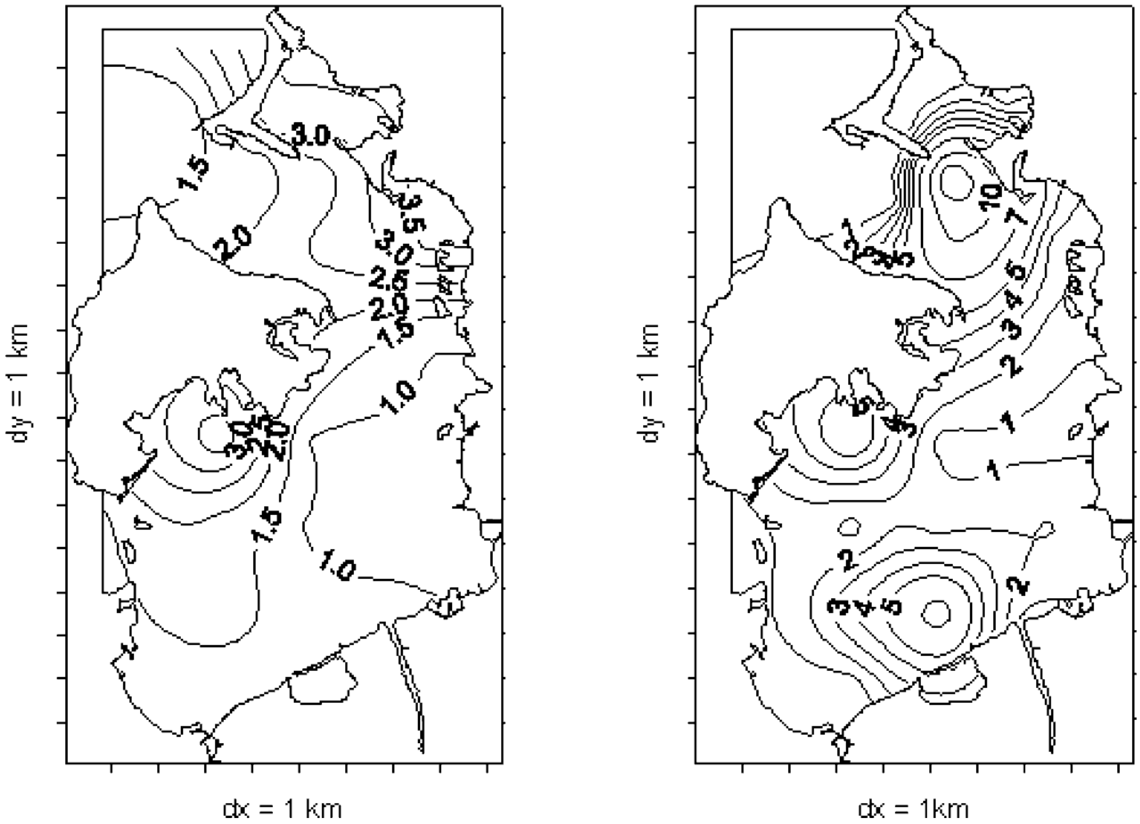
(a) **(b)**

Fig. 2.5. Contents of dissolved oxygen (ml/liter) in waters of the bottom layer of the Cartagena Bay for the dry (a) and wet (b) seasons of a year according to the data of monitoring for 1996–1999.

The wind conditions in the bay are characterized by the predominance of strong (with daily average velocities of up to 8 m/sec) northeast trade winds in the dry period of a year (January–May) and weak (up to 3 m/sec) winds during the rainy season (August–November).

In the rainy season, the flow rate of the Dique Channel is maximum and the vertical turbulent exchange is minimum (due to the absence of strong winds). This leads to the formation of a sharp pycnocline in the subsurface layer of the bay blocking the processes of mass and gas exchange between the surface and bottom layers. The biogenic substances coming both with the waters of the Dique Channel and from the anthropogenic sources are distributed inside the surface freshened layer. In the major part of the water area of the bay, due to the low transparency of waters, the productivity of phytoplankton is limited by illuminance. However, near the straits, where the transparency of waters increases as a result of the gravitational sedimentation of the suspension and dilution with pure waters of the sea, we detect local sites of high productivity and biomass of phytoplankton.

After dying, the organic substances of autochthonous origin formed as a result of the photosynthesis of phytoplankton move down into the deeper layers under the action of gravitational forces and suffer biochemical destruction by bacteria. The oxygen dissolved in seawater is spent for the oxidation of inert organic matter and nitrification.



(a) **(b)**

Fig. 2.6. Typical distributions of BOD_5 (mg/liter) in the surface (a) and bottom (b) layers of the Cartagena Bay for the rainy season plotted according to the data of monitoring for 1996–1999.

The morphological specific features of the analyzed basin (shallow-water straits in combination with a great depth of the bay), weak vertical turbulent water exchange, and the absence of photosynthetic production of oxygen below the pycnocline result in the formation of a deficiency of oxygen in the bottom layer of the bay (Fig. 2.5). The aerobic hydrochemical conditions formed in waters of the bottom layer in the major part of the water area of the bay are replaced by the anaerobic conditions, which leads to the death of aerobic organisms, deceleration of the processes of biochemical destruction of inert organic matter, and hence, to the accumulation of nondestructed organic matter in the bottom layers (Fig. 2.6).

In January (after the rainy season), the flow rate of the Dique Channel is minimum, the subsurface pycnocline becomes weaker and the wind-induced mixing of waters and the vertical turbulent exchange between the subsurface photic and bottom layers of the bay are intensified. As a result, the oxygen content of the bottom layer increases to 2–3 mliter/liter (Fig. 2.5a).

Thus, the action of high anthropogenic loads (caused by the industrial and anthropogenic sources of pollution) upon the ecosystem of the Cartagena Bay and the inflow of polluted waters of the River Magdalena result, together with the morphological features of the basin, in the eutrophication of waters in the bay and periodic formation of the deficiency of oxygen in the bottom layer. Since these processes are caused by a complex family of natural and anthropogenic factors, it is practically impossible to evaluate the efficiency of various nature-preservation measures aimed at the improvement of the current ecological situation without using mathematical models of the quality of water.

The data of ecological monitoring also show that the level of pollution of water with pathogenic bacteria in the Cartagena Bay is fairly high and exceeds the existing permissible limits for the zones of primary contact of human beings with water [165]. The concentration of Coliform bacteria in waters of the bay is determined by numerous natural factors (temperature, salinity, and transparency of water, storm discharge, flow rate of the channel, etc.) whose relative roles vary during a year. The municipal sewage waters of the city are the main source of pollution. As shown in [165], high concentrations of the Coliform bacteria should be expected during the period of intense storm precipitation, when the flow of polluted waters through the system of storm discharge and sewerage becomes much more intense and the concentration of pathogenic bacteria in these waters increases due to the washout of formerly isolated sources of pollution inside the city. Sometimes the waters of the Dique Channel also make a significant contribution to the pollution of waters in the bay with pathogenic microflora.

2.1.2. Shallow-Water Tropical Ciénaga-de-Tesca Lagoon

The shallow-water Ciénaga-de-Tesca Lagoon is located to the northeast of the city of Cartagena (Figs. 2.2 and 2.3). The shape of the lagoon resembles a triangle elongated in the south–north direction for 7 km. Its width in the south part reaches ≈ 4.5 km. At the same, in the north part it does not exceed several hundred meters. The area of water surface of the basin is $\approx 22.5\,\text{km}^2$, its average depth is ≈ 0.85 m, and the maximum depth reaches 1.6 m (Fig. A.2).

The lagoon periodically communicates with the Caribbean Sea through a strait located in its north part. The depth of the strait does not exceed 1 m and its width is ≈ 100 m. The strait is open during the rainy season (August–November) and closed in the dry period of a year (January–April).

The water balance of the lagoon is formed as a result of water exchange with the sea, evaporation, atmospheric precipitation in the wet period of a year, and the inflow of fresh waters from the natural streams and the sewage system of the city of Cartagena.

At present, according to numerous parameters of the quality of water (e.g., BOD_5 and the content of PO_4^{3-}), the Ciénaga-de-Tesca Lagoon can be regarded as a very dirty (hypertrophic and polysaprobic) basin [62] with all symptoms of eutrophication, including the supersaturation of waters of the surface layer with oxygen and its complete absence in the bottom layer at depths greater than 1 m. The role of the main source of pollution is played by the sewer pipes delivering about 60% of the daily amount of crude industrial and municipal sewage waters of Cartagena into the lagoon. The location of these sources and their characteristics are presented in Fig. 2.7 and in Table B.3.

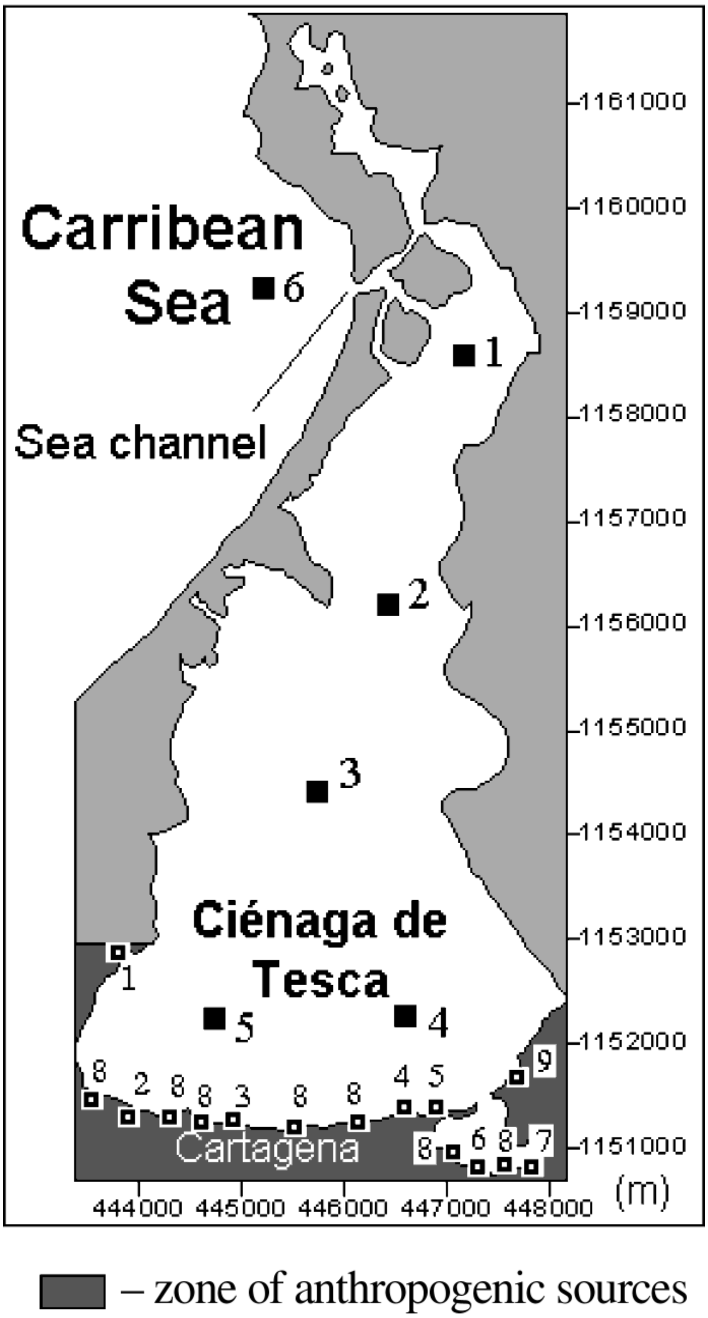


Fig. 2.7. Schematic map of the Ciénaga-de-Tesca Lagoon with locations of the anthropogenic sources of pollution (see Table B.3). The points of monitoring carried out in 1996–1998 are marked by the squares.

In view of the fact that the south most polluted part of the water area of the Ciénaga-de-Tesca Lagoon is located inside the city of Cartagena and near its recreational zone, the problem of restoration of the ecosystem of this basin seems to be quite urgent.

In order to develop scientifically grounded nature-preservation measures aimed at the improvement of the ecological situation, a systematic ecological monitoring of the quality of waters was carried out in the Ciénaga-de-Tesca Lagoon in 1996–1999 [159, 162].

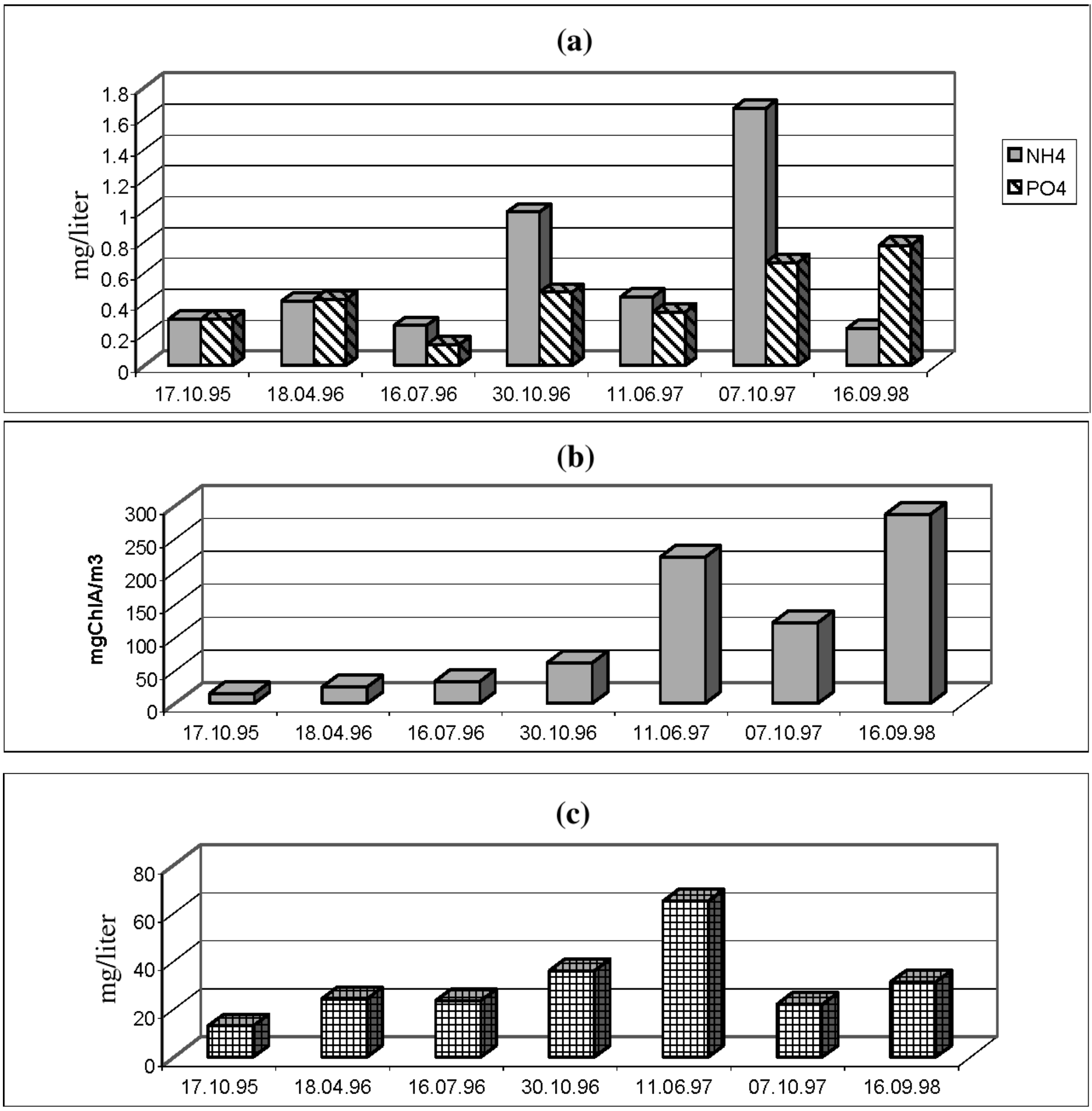


Fig. 2.8. Variability of the concentrations of nitrogen of ammonium and phosphorus of phosphates (a), chlorophyll A (b), and BOD (c) averaged over the area of the basin in waters of the Ciénaga-de-Tesca Lagoon according to the data of monitoring carried out in 1995–1998.

The complex of observations included the determination of both hydrological (transparency, temperature, and salinity of waters) and hydrochemical (NH_4^+, NO_2^-, NO_3^-, PO_4^{3-}, BOD_5, and O_2) characteristics. However, due to the organizational and financial difficulties, specialized hydrobiological observations were not included in the program of monitoring. The biotic component of the ecosystem was studied in the course of monitoring only in the form of evaluation of the concentrations of chlorophyll A and Coliform bacteria.

The typical values of the hydrochemical parameters at different points of the water area of the lagoon obtained as a result of averaging of the data of observations over the entire period of monitoring are summarized in Table 2.2.

Table 2.2. Typical Values of the Ecological Characteristics of State of the Ciénaga-de-Tesca Ecosystem Obtained as a Result of Averaging of the Data of Monitoring for 1996–1998. The Location of the Stations Is Shown in Fig. 2.7

Number of station	S, ‰	pH value	Transparency, m	PO_4^{3-}, mgP/liter	NH_4^+, mgN/liter	NO_2^-, mgN/liter	NO_3^-, mgN/liter	BOD_5, mg/liter	O_2, ml/liter	B_f, mgChlA/m^3
1	24.8	8.55	0.27	0.48	0.49	0.015	0.43	15.8	5.2	71.4
2	24.2	8.76	0.28	0.53	0.43	0.010	0.46	17.9	5.7	100.7
3	23.6	8.83	0.28	0.54	0.56	0.009	0.51	16.9	5.9	77.7
4	22.1	8.85	0.23	0.63	0.63	0.011	0.38	24.8	6.5	122.8
5	22.7	8.84	0.22	0.56	0.58	0.012	0.46	24.7	6.1	107.4
6	33.0	8.40	1.3	0.05	0.20	0.036	0.29	6.9	3.9	14.9
Mean value	23.4	8.77	0.26	0.54	0.55	0.011	0.45	20.3	5.90	96.1
Standard deviation	9.1	0.56	0.06	0.22	0.53	0.008	0.78	11.8	2.79	79.2

Comparing these results with the archival data of episodic observations performed in 1983–1984 and 1994–1995, we see that the quality of waters in the lagoon significantly deteriorated and the biotic component of its ecosystem passed into a qualitatively new state. Thus, the average BOD value increased from 14 to 30 mg/liter and the concentration of chlorophyll A from 12 to 100 mg Chl.A/m^3 and even more. Moreover, we observe an increase in the amplitudes of oscillations of the mean (over the area of the basin) values of the concentrations of mineral compounds of biogenic elements. Together with the stable growth of the concentration of chlorophyll A, this may serve as an indication of the violation of balance between the production and destruction processes formed earlier and the instability of the dynamics of the ecosystem. The development of an event of El Niño in 1997 (as a result of which the indicated year was climatically anomalous in numerous meteorological parameters) could also be responsible for the violation of balance. The dynamics of transition of the Ciénaga-de-Tesca ecosystem into a qualitatively new state in 1995–1998 is illustrated in Fig. 2.8.

Thus, the results of monitoring reveal a sharp worsening of the ecological situation in the analyzed basin and urgent necessity of undertaking nature-preservation measures for its improvement.

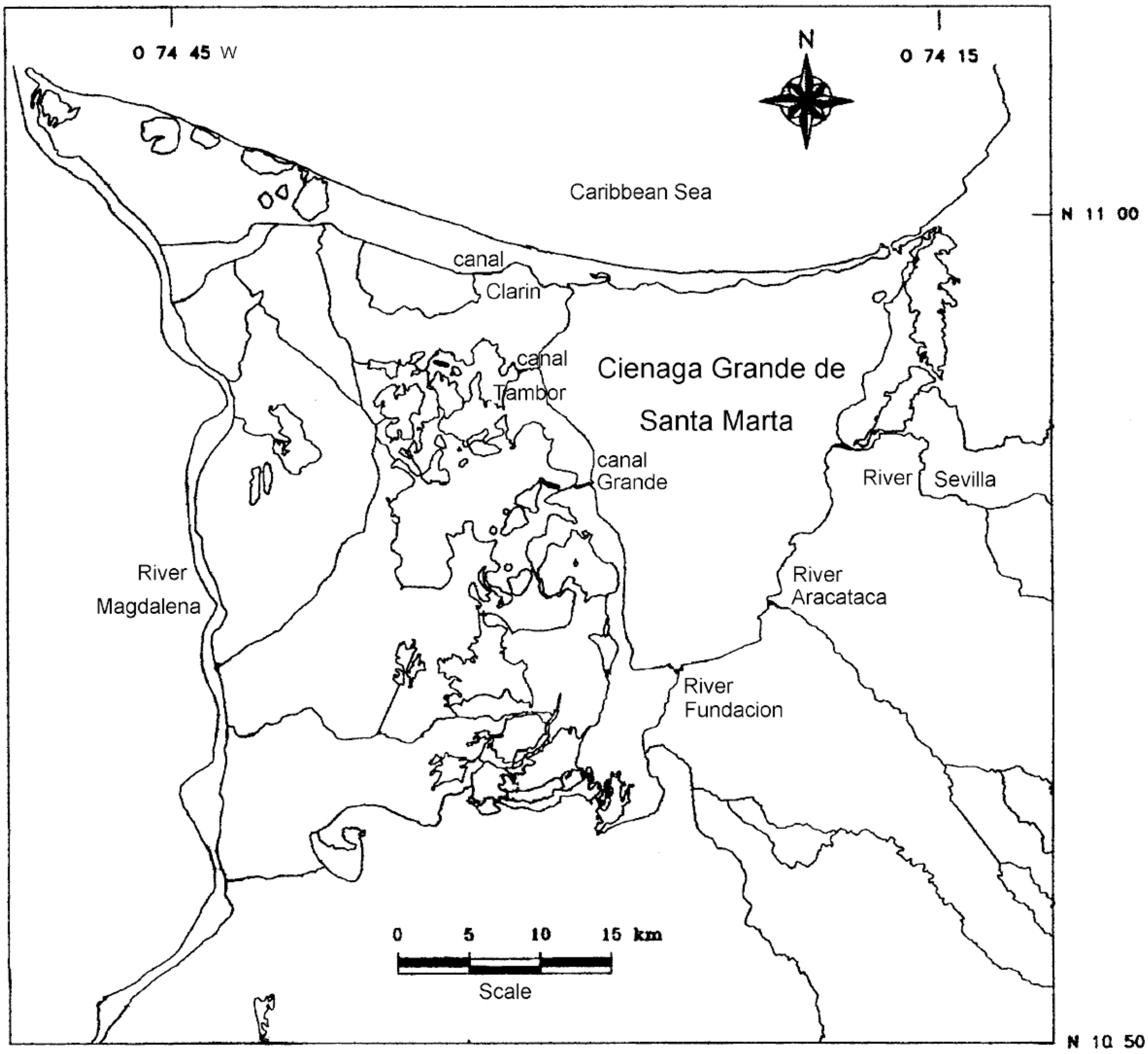


Fig. 2.9. Schematic map of the Ciénaga-Grande-de-Santa-Marta Firth and the system of lakes and channels connecting it with the Magdalena River and Caribbean Sea.

The efficiency of various scenarios of control over the quality of water in the basin can be evaluated only on the basis of the results of prognostic numerical simulations performed by using mathematical models.

2.1.3. Ciénaga-Grande-de-Santa-Marta Shallow-Water Tropical Estuary-Type Basin

The Ciénaga-Grande-de-Santa-Marta Firth is a shallow-water tropical lagoon artificially transformed into an estuary-type basin. The firth occupies a part of the Caribbean coast of Colombia bounded between 10°44′–11°00′ N and 74°19′–74°31′ W (Fig. 2.9). The area of the water surface of the basin constitutes $423\,km^2$ and its average depth is equal to $1.6\,m$ (Fig. A.3). At the north boundary, the firth communicates with the Caribbean Sea through the Boca-de-la-Barra Strait $\approx 280\,m$ in width. As a rule, the seasonal oscillations of the water level in the firth vary within the range 30–50 cm. We also observe the semidiurnal tidal oscillations of the level whose amplitude is equal to 20–40 cm in the neighboring part of the sea and ≈ 7 cm inside the firth.

The Sierra-Nevada-de-Santa-Marta Mountains neighbor the firth on its east and southeast boundaries. The small Frío, Sevilla, Aracataca, Fundación, and Aji Rivers flow down from these mountains into the firth. The water-catchment area of these rivers is characterized by extensive agricultural activities. On the west boundary, the firth neighbors the Pajarales complex of small lakes connecting it with the large Magdalena River through a system of channels.

This enables us to conclude that the quality of waters in the firth is formed under the influence of the discharge of small rivers, water exchange with the sea through the strait, and the inflow of waters of the Magdalena River through the system of artificial channels and natural lakes of the Pajarales complex. Among these factors, the predominant role is played by the inflow of waters from the Magdalena River and water exchange with the sea.

The water area of the firth is also characterized by the presence of objects of industrial cultivation of oysters and shrimps. Moreover, the firth, together with the neighboring system of lakes, form a highly productive ecological system of extremely high importance as a region of fishery for the inhabitants. The rate of primary production of the organic matter by phytoplankton in small lakes is equal to $0.4\ \mathrm{gC}/(\mathrm{m}^2\cdot\mathrm{h})$. The water area of the firth and at its coasts are partially occupied by unique mangrove thickets.

The currently existing hydrochemical conditions in the firth were formed artificially. In the early 1980s, as a result of the construction of a motorway along the sea shore, the natural water exchange of the Pajarales system of small salt lakes with the sea was violated. This led to a strong salinization of these lakes and, hence, to the mass death of unique perennial mangrove thickets on their coasts. In the early 1990s, to decrease the salinity of waters in the lakes, the existing channels were reconstructed (deepened and broadened) and additional channels connecting the firth with the Magdalena River via the system of salt lakes were constructed.

As a result of the inflow of river waters, the salinity of waters strongly decreased not only in the small lakes but also in the firth itself. The level of eutrophication of the basins significantly increased. The excessive freshening of waters of the Ciénaga-Grande-de-Santa-Marta Firth created unfavorable living conditions for the marine organisms among which oysters and shrimps should be mentioned especially. The process of freshening in the system of salt lakes, on the one hand, promotes the increase in the catch of valuable species of freshwater fishes but, on the other hand, creates favorable conditions for the growth of new (lower than earlier) species of mangroves. In the wet period, as the level of water increases, they are flooded and die delivering additional amounts of inert organic matter to the waters of the firth, thus increasing their trophity and saprobity.

This enables us to conclude that the problems of prediction of the productivity of the ecosystem of the Ciénaga-Grande-de-Santa-Marta Firth and control over the quality of its waters are quite urgent.

The complex ecological monitoring of the Ciénaga-Grande-de-Santa-Marta Firth has been carried out since the mid-1980s. However, only since 1993 (after the reconstruction of the connecting channels), the indicated monitoring became systematic. The complex of observations included monthly evaluation of the following hydrochemical and hydrological parameters: NH_4^+, NO_2^-, NO_3^-, PO_4^{3-}, O_2, chlorophyll A, organic seston, and the transparency, temperature, and salinity of water. In addition, specialized hydrobiological experiments aimed at measuring the production of phytoplankton depending on the concentrations of biogenic elements, transparency of water, the biomass of phyto- and zooplankton, and the amount of bacteria were performed episodically. The fluxes of mineral nitrogen and phosphorus from the bottom sediments into the bulk of water were also experimentally evaluated.

Table 2.3. Typical Values of the Ecological Characteristics of State of the Ciénaga-Grande-de-Santa-Marta Ecosystem for Different Periods of Monitoring and in the Extreme Years

Years	NH_4^+, mgN/liter	NO_2^-, mgN/liter	NO_3^-, mgN/liter	PO_4^{3-}, mgP/liter	B_f, mgChlA/ m^3
1987–88	0.01	0.005	0.008	0.03	65
1994	0.10	0.007	0.030	0.25	550
1995–96	0.02	0.005	0.035	0.07	140
1993–99	0.06	0.006	0.040	0.09	240

The main disadvantage of the outlined procedure of ecological monitoring is connected with the absence of measurements of the amount of inert organic matter (which should be regarded as one of the main abiotic components of the water ecosystem) in waters of the firth. The concentration of inert organic matter was evaluated according to the parameters of BOD, oxidizability with $KMnO_4$, and the fraction of detritus in seston beginning with the second half of 1999.

Another serious problem encountered in the application of the data of monitoring for the ecosystem analysis of the conditions of formation of the quality of waters in the firth is connected with the fact that the hydrobiological observations were, for the most part, carried out prior to the onset of reconstruction of the system of connecting channels and development of the process of eutrophication of the basin.

The analysis of the data of monitoring shows that the reconstruction of the channels resulted in the increase in the concentration of mineral nitrogen in waters of the firth and, hence, in a strong weakening of its influence as a factor limiting the primary production of organic matter by phytoplankton (Table 2.3). Under the currently existing conditions, the role of the main limiting factors is played by the low transparency of waters and, possibly, by the influence of salinity of waters on the functional activity and mortality of various kinds of algae.

Table 2.4. Typical Values of the Parameters of Quality of the Ciénaga-Grande-de Santa-Marta Waters, Sea Waters in the Neighboring Water Area of the Caribbean Sea, and Waters of the External Sources (Inflows)

Parameters	Typical values							
	CGSM	Sea	r. Fundación	r. Aracataca	r. Sevilla	Clarin channel	Tambor channel	Grande channel
Temperature, °C	30.	26.	31.	31.	31.	30.	30.	30.
Salinity, ‰	20.	35.	0.	0.	0.	0.	0.	0.
Transparency, m	0.4	1.0	0.2	0.1	0.15	0.2	0.3	0.4
Phosphates PO_4^{3-}, mgP/liter	0.09	0.05	0.30	0.35	0.35	0.09	0.07	0.12
Ammonium NH_4^+, mgN/liter	0.06	0.02	0.10	0.04	0.10	0.04	0.05	0.08
Nitrites NO_2^-, mgN/liter	0.006	0.003	0.01	0.01	0.01	0.009	0.006	0.01
Nitrates NO_3^-, mgN/liter	0.04	0.09	0.10	0.20	0.19	0.06	0.04	0.15
Oxygen O_2, mg/liter	6.	5.0	1.1	3.2	0.9	4.0	4.5	5.0
Inert organic matter, mg O_2/liter	20.	12.0	17.0	16.0	15.0	20.0	19.0	20.0
Phytoplankton, mgChlA/m^3	240.0	40.0	60.0	10.0	40.0	120.0	160.0	250.0
Bacterial plankton, mgC/m^3	1300.	1000.	1400.	1400.	1400.	1300.	1300.	1300.
Zooplankton, mgC/m^3	3400.	2500.	2000.	2000.	2000.	2500.	3600.	3600.

Note that, in the 1980s, the average concentration of chlorophyll A was equal to 70 mgChlA/m^3. In the 1990s, it became as high as 200–250 mgChlA/m^3. Although the concentration of phosphates increased from 0.03 to 0.09 mgP/liter, its actual influence on the productivity of the ecosystem was insignificant because, even in the 1980s, this concentration exceeded the needs of phytoplankton.

Table 2.5. Flow Rates of Small Rivers (m^3/sec) in Different Seasons of a Year (Data of the Colombian Institute of Hydrology, Meteorology, and Environmental Research)

Rivers	Dry season (March)	Short rainy season (May)	Short dry season (July)	Rainy season (October)
Fundación	11.4	70.0	25.0	38.0
Aracataca	1.3	1.5	3.0	7.0
Sevilla	6.6	86.0	20.0	61.0
Aji	0.5	1.0	0.5	2.0

Table 2.6. Elevations of the Water Level (m) on the Outer Boundaries of the Channels Connecting the System of Small Lakes with the Firth [151]

Channels	Dry season (March)	Short rainy season (May)	Short dry season (July)	Rainy season (October)
Grandle	–0.03	0.06	0.02	0.17
Clarin	–0.11	0.04	0.02	0.23
Tambor	–0.05	0.07	0.02	0.18

The chemical and biological characteristics of the quality of river, sea, and firth waters according to the data of the ecological monitoring of 1993–2000 are presented in Table 2.4. In Tables 2.5 and 2.6, one can find the flow rates of the investigated small rivers and the elevations of water level in the connecting channels over the sea level for different seasons of the year (Fig. 2.9).

As follows from Table 2.6, the water levels in small lakes in the dry season are lower than the sea level and, hence, we observe the maximum inflow of waters from the sea into the firth and through the channels into the lakes. On the contrary, in the rainy season, the inflow of waters from the Magdalena River is maximum and, therefore, we can expect the deterioration of the quality of waters in the firth in this period.

2.2. Water Areas of the Northwest Part of the Black Sea

2.2.1. Dnieper–Bug and Odessa Regions

The Dnieper–Bug estuary region is located in the north part of the northwest shelf of the Black Sea from the Kinburnskii Strait to the coasts of Odessa (Fig. 2.1). There are two predominant forms of the bottom topography in the Dnieper–Bug estuary region: the Dnieper Paleovalley and the Odessa Bank. The Dnieper Paleovalley continues the river bed along the bottom of the sea (first in the latitudinal direction) stretching in the form of a narrow 5-km trough along the coast from the Dnieper–Bug firth westward and separating the Odessa Bank from the littoral slope. Near the west end of the bank, the Dnieper trough takes the meridional direction, becomes wider, and forms (to the south) the Odessa Depression with depths greater than 25 m. Near the Sukhoi Firth, we observe one more positive form of the bottom topography, namely, a small Il'ichevsk elevation with depths less than 20 m. The maximum depth of this region is is equal 28 m and the average depth to 14 m (Fig. 3.4).

The description of specific features of the hydrological and hydrochemical conditions formed in the Dnieper–Bug estuary region in the northwest part of the Black Sea can be found in [20, 33–35, 79, 103, 106].

The Odessa region of the northwest part of the Black Sea belongs to the Dnieper–Bug estuary region [9]. The quality of waters in this region of the sea is determined, on the one hand, by the inflow of biogenic substances and pollutants with the river discharge of Dnieper and Yuzhnyi Bug and, on the other hand, by the sewage waters of the anthropogenic sources of pollution located in the coastal zone. The industrial, harbor, and municipal complexes of the cities of Odessa, Il'ichevsk, and Yuzhnyi operating on the sea coast in this region are the sources of sewage waters containing large amounts of biogenic substances, synthetic surfactants, oil products, and other substances polluting marine media [54, 104].

The Odessa region of the northwest part of the Black Sea is a zone of great recreational importance because its coast is occupied by beaches, seaside resorts, and sanatoria. Moreover, this water area neighbors the Odessa Bank—one of the most valuable regions of fishery in the Black Sea (the region of intense reproduction of fish). Therefore, the analysis of the roles of anthropogenic sources and river discharge in the formation of the current level of pollution and eutrophication of waters in this region of the northwest part of the Black Sea, as well as the prediction and control of the quality of its waters are urgent problems of management of the marine resources and preservation of nature. It is impossible to solve these problems without using the mathematical models of the quality of waters in the sea taking into account both the phenomena of hydrodynamic dilution of river and sewage waters and the chemical and biological processes of transformation of pollutants and biogenic substances in marine media.

In 1988–1999, the Odessa Branch of the Institute of Biology of Southern Seas realized an extensive program of complex ecological monitoring of the sea area near the coasts of Odessa and its satellite towns (Il'ichevsk and Yuzhnyi). The accumulated results made it possible to establish and describe the specific features of the behavior of hydrological conditions [34, 35, 106], circulation of waters [35, 99, 100], and hydrochemical conditions in this water area [33, 79, 106].

For the indicated period, 31 complex survey of the water area with the total number of stations equal to 557 were carried out in the Odessa region of the northwest part of the Black Sea. The number of surveys varied from one to six per year. The number of stations in these surveys varied from 16 to 42 (and the average number was equal to 27). In most cases, the annual cycle of monitoring included two surveys corresponding, respectively, to the spring hydrological season (April–May) and the second half of the summer season (August–September). In total, three surveys were performed in April, nine in May, one in July, nine in August, two in September, two in October, three in November, one in December, and one in February.

The program of monitoring was realized in order to analyze the quality of marine media in the Odessa region of the northwest part of the Black Sea and included the determination of both the standard hydrological (temperature and salinity) and hydrochemical (contents of biogenic substances, dissolved oxygen, etc.) characteristics of waters in the surface and bottom layers and the concentration of various kinds of pollutants.

Since 1992, the program of observations included the evaluation of the concentration of chlorophyll A. The quantitative samples of phytoplankton were taken at some stations in May and August 1994–1995, in May and October 1996, in September 1997, and in May and August 1998. Note that the amount of available data of these hydrobiological investigations is quite small. However, together with the results of fairly regular seasonal surveys of the hydrological and hydrochemical parameters, they enable us to study the influence of some hydrological phenomena on the formation of the current level of trophity of waters and oxygen conditions in the investigated water area.

The results of 12-yr ecological monitoring enable us to establish the following characteristic features of the formation of hydrological and hydrochemical conditions in waters of the Odessa region of the northwest part of the Black Sea:

— the predominance of wind currents for the most part of the year and the influence of the Odessa Bank on the character of circulation of waters;

— the seasonal variability of the degree of influence of freshwater discharge of the Dnieper and Yuzhnyi Bug Rivers on the hydrological structure, dynamics, and hydrochemical parameters of the quality of waters;

— the presence of significant anthropogenic sources of eutrophication and pollution of marine media in the costal zone of this region;

— the presence of systematic events of wind-induced coastal upwelling guaranteeing the possibility water and mass exchange between the surface and bottom layers of the water area in spring and summer when these layers are separated by a sharp seasonal pycnocline.

In the annual course of the temperature and salinity of waters in the Odessa region of the northwest part of the Black Sea, it is customary to distinguish the following hydrological seasons: spring (April–June), summer (July–September), autumn (October–December), and winter (January–March). March is regarded as a winter month due to the low temperature of water and June is regarded as a spring month due to the low salinity of water (although the temperature of water in June is fairly high and can be regarded as typical of summer).

In spring, the vertical thermohaline structure of waters is formed under the influence of river discharge and heating of water. The processes of freshening and simultaneous heating of the surface layer lead to the formation of a subsurface layer characterized by the jump of density. Indeed, the temperature of water in the surface layer at the beginning of spring is equal to 7–9°C, in May to 13–15°C, and in June to 18–19°C. As a rule, the temperature of the bottom layer constitutes 4–5°C at the beginning of spring and increases to 7–8°C at the end of this season. The salinity of the surface layer near the north coast decreases to 6–11‰ at the peak of high water and then rises to 13–15‰ at the end of spring. In the bottom layer, the level of salinity of waters varies within the range 15–17‰ in the deep-water part of the analyzed region and may decrease to 9–11‰ in the shallow-water part of the region as a result of mixing.

In summer, as a result of weakening of the river discharge and the general intensity of circulation, the waters of the subsurface layer become much more unstable. The presence of a layer with density jump in the analyzed region in this period is explained, first of all, by the action of thermal factors. As a result, even a weaker (as compared with spring) wind action leads to a greater deepening of the boundary of the upper mixed layer in summer. Note that the process of deepening of the upper mixed layer runs during the periods of strong winds, which are also observed in summer (but less frequently than in spring). The presence of relatively weak winds is sufficient to support the existence of the already formed upper mixed layer. In summer, the upper boundary of the layer with density jump moves down to a depth of 7–10 m. In the surface layer, the temperature of water is equal to 21–24°C and, in the bottom layer, varies within the range 8–10°C in the deep part of water area and 17–22°C in the shallow-water zones. The level of salinity of the surface waters varies within the range 14–17‰. In the bottom layer, it is equal to 16–17.5‰. In the absence of offshore winds, the distributions of temperature and salinity of water in the surface layer are spatially homogeneous.

In autumn, the process of intense cooling of waters accompanied by the intensification of winds promotes active convective and wind mixing and, as a final result, leads to the destruction of vertical stratification. Indeed, in October, the temperature of the surface layer of water is equal to 15–17°C and decreases to 6–8°C in December. As the river discharge increases, the level of salinity of waters in the surface layer decreases. At the end of autumn, in the presence of active wind mixing, the values of temperature and salinity in the bulk of water are equalized and, as a result, the entire analyzed water basin is occupied by a single mass of water with a temperature of 8–9°C and a salinity of 16.5–17‰.

The degree of influence of the river discharge on the hydrological and hydrochemical conditions in the Odessa region is determined both by the seasonal variability of the flow rates of Dnieper and Yuzhnyi Bug and by the predominant winds.

At the exit of the Dnieper–Bug Firth, the river waters spread over the sea surface (in a thin layer) in the form of a tongue oriented, depending on the wind, in two possible directions. Thus, in the case where the north and northwest winds are predominant, the axis of the tongue is directed to the southwest and the process of freshening is not observed near the coasts of Odessa. In this case, the level of salinity of waters in the analyzed region varies within the ordinary range 14–16‰. In the second (fairly frequently observed) case of spreading, the tongue of freshened water stretches westward over the Odessa Bank and along the north coast of the northwest part of the Black Sea, reaches Odessa, and significantly decreases the level of salinity of waters in the surface layer. This type of spreading is especially well visible in April–May in the presence of strong southeast and east winds when, according to the data of the Odessa-Harbor station, the level of salinity of waters decreases to 10–12‰ and, in exceptional cases, even to 3‰ [21]. Parallel with the already described two types of spreading, the river waters at the exit of the firth may spread in the form of a fan. In these cases, the flow from the Kinburnskii Strait spreads over the sea surface in the radial direction and fairly rapidly disappears. This means that the firth water rapidly transforms into seawater (as far as the level of salinity is concerned). The length of the zone of transformation of river waters does not exceed 20 km and the level of salinity of waters in the Odessa region of the northwest part of the Black Sea does not decrease in this case [9].

In the Dnieper–Bug estuary region, the winds of north directions are predominant for the whole year. According to the data of the Odessa-Harbor station, their total repeatability constitutes 43% [21]. However, in the spring period (April–May), it is typical to observe a certain weakening of the winds of north directions (to 36%) and strengthening of the southeast (22%) and south (17%) winds promoting the penetration of the tongue of transformed river waters into the Odessa region. Moreover, according to [6], the repeatability of storm winds (with velocities ≥ 15 m/sec) of the east directions near the north coast close to the Grigor'evskii Firth is more than four times higher than the repeatability of the winds of west directions.

In view of the fact that the flow rate of the Dnieper is maximum in May, we can conclude that the penetration of the tongue of transformed waters of the Dnieper and Yuzhnyi Bug Rivers into the Odessa region is most probable at the end of spring. This is confirmed by the data of observations over the level of salinity at the Odessa-Harbor station [28] and the results of hydrological surveys of the Odessa Branch of the Institute of Biology of Southern Seas carried out in 1988–1999. As for the nine surveys carried out in May, the tongues of freshened waters of different intensities were observed near the north coast of the investigated region in May 1988, 1994–1996, and 1998 and in April 1990.

Since significant amounts of organic and mineral compounds of biogenic elements penetrate with river waters into the Dnieper–Bug Estuary Region in the northwest part of the Black Sea, it is natural to expect that the appearance of the tongue of transformed river waters in the Odessa region promotes the growth of production and biomass of phytoplankton and the increase in the role played by freshwater species in its formation. Note that the results of monitoring show that the indicated effect of river discharge indeed takes place (Figs. 2.10 and 2.11). As a rule, high concentrations of chlorophyll A and the biomass of phytoplankton correspond to the tongue of freshened waters.

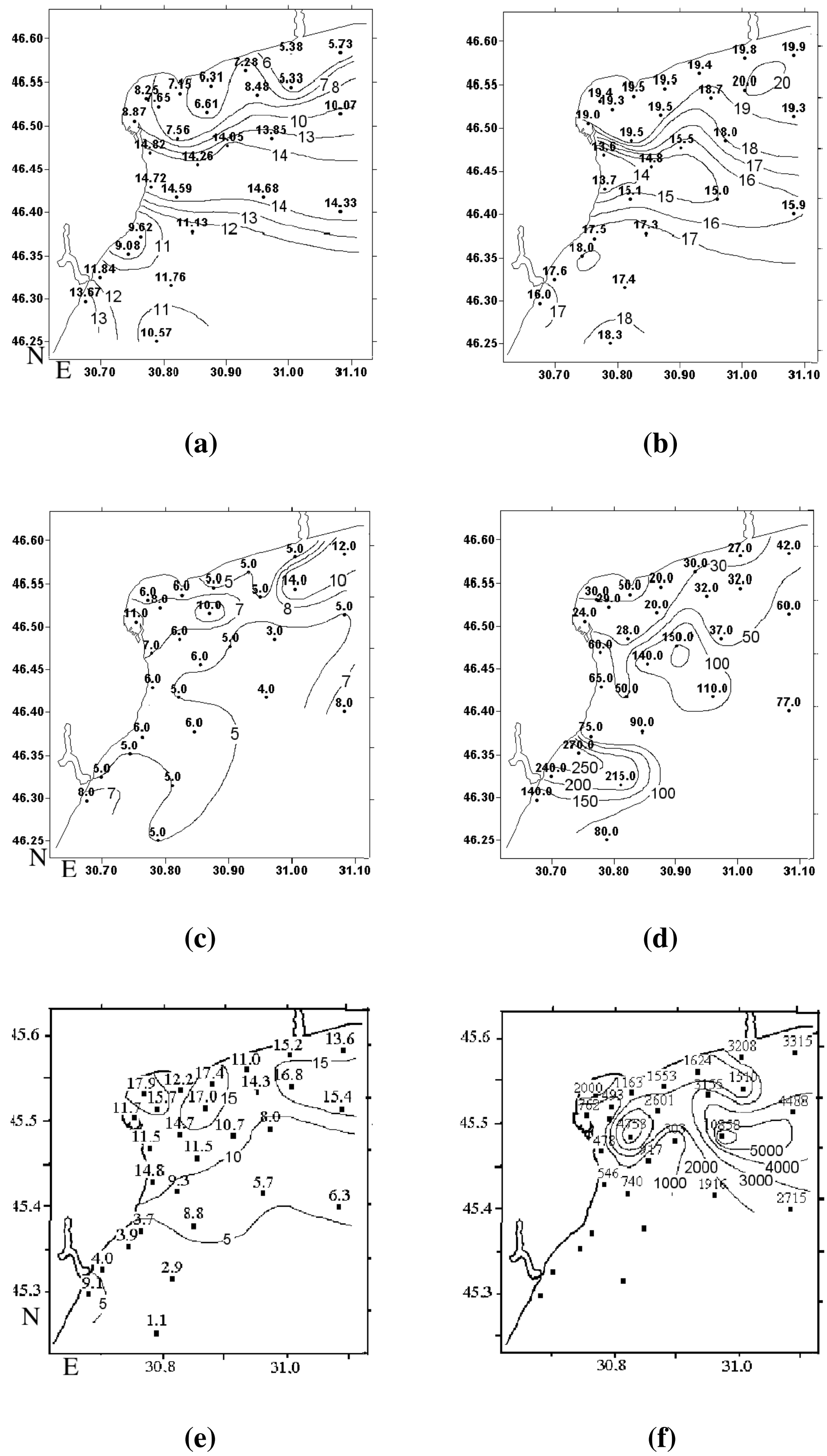


Fig. 2.10. Space distributions of various parameters over the surface layer of the Odessa region in the northwest part of the Black Sea (May 1994): (a) salinity of water (‰), (b) temperature of water (°C), (c) phosphorus of phosphates (μgP/liter), (d) nitrogen of ammonium (μgN/liter), (e) chlorophyll A (mgChl A/m^3), (f) biomass of phytoplankton (mg/m^3).

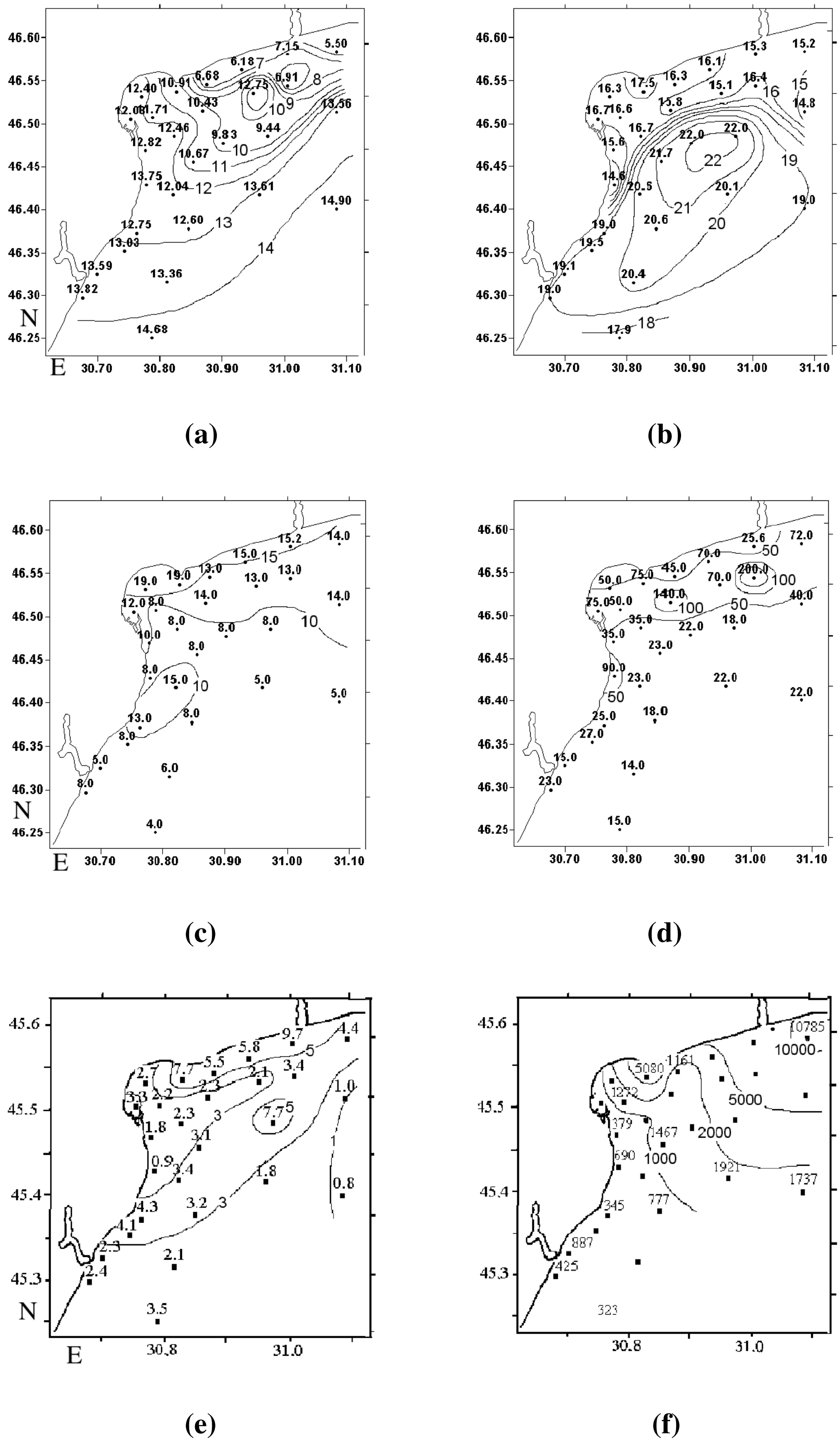


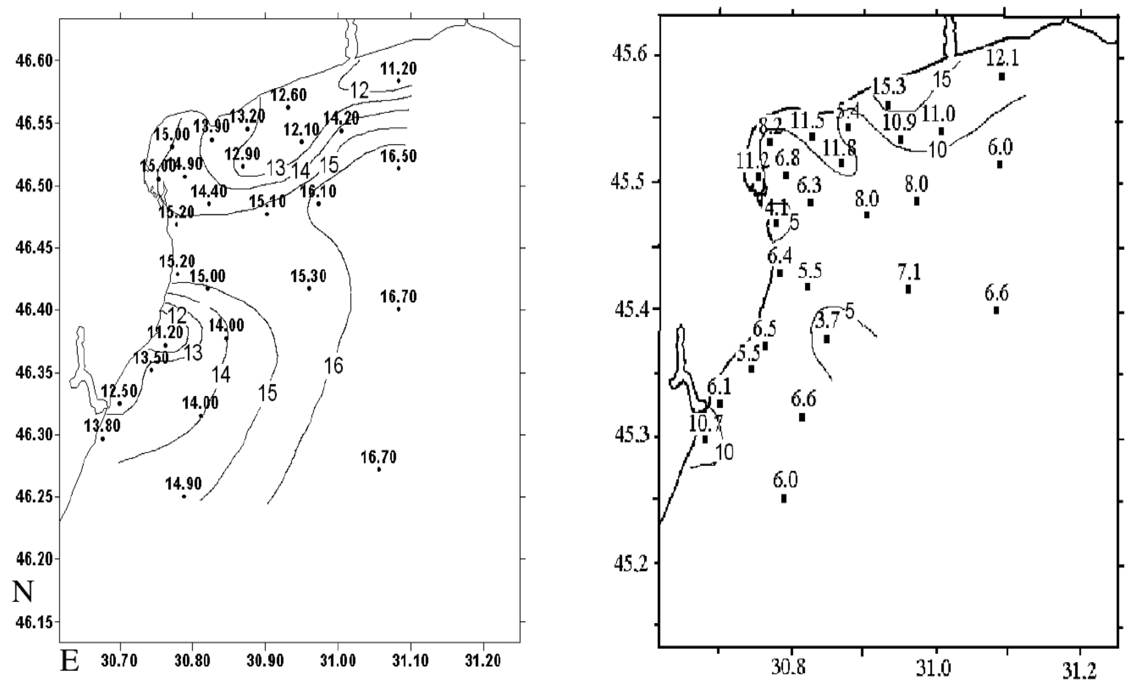
Fig. 2.11. Space distributions of various parameters over the surface layer of the Odessa region in the northwest part of the Black Sea (May 1995): (a) salinity of water (‰), (b) temperature of water (°C), (c) phosphorus of phosphates (μgP/liter), (d) nitrogen of ammonium (μgN/liter), (e) chlorophyll A (mgChl A/m^3), (f) biomass of phytoplankton (mg/m^3).

The influence of penetration of transformed river waters into the analyzed water area on the space distributions of biogenic elements is ambiguous Thus, in May 1995, the elevated concentrations of mineral compounds of nitrogen and phosphorus corresponded to the tongue of freshened waters near the north coast of the investigated region. At the same time, in May 1994, the concentrations of phosphates in the region of the tongue were also high but the concentrations of ammonium nitrogen were minimum over the entire water area.

To explain this ambiguity, it is necessary to take into account the fact that the current concentrations of the mineral compounds of biogenic elements observed in the course of the surveys depend not only on their penetration from the outside (in particular, with river discharge) but also on the ratio of the intensities of their utilization in the processes of photosynthesis and regeneration (in the course of mineralization of the organic matter). Hence, in each specific case, the character of variability of the concentrations of mineral compounds of biogenic elements in the tongue of freshened waters and their ratios depend not only on the characteristics of river discharge but also on the temperature and transparency of waters, the phase of development of the plankton community, etc.

Thus, the comparative analysis of the already presented results of spring surveys of 1994 and 1995 (Figs. 2.10 and 2.11) shows that, as follows from the concentrations of chlorophyll A, phosphates, and ammonium and the character of space distribution of the biomass of phytoplankton in the tongue of freshened waters, the rates of utilization of biogenic elements by phytoplankton in the process of photosynthesis were higher in 1994. Therefore, the resource of mineral compounds of biogenic elements transformed into the resource of organic matter. It seems likely that the elevated temperature of water recorded in the tongue of freshened waters in 1994 (as compared with the survey of 1995) could be responsible for this phenomenon. Moreover, according to the data of hydrobiological investigations [70, 93], during the period of water blooming in the spring season of 1994, the freshwater species constituted 34.2% of the average biomass of phytoplankton. At the same time, in spring 1995, the contribution of these species to the formation of the biomass of algae was half as large (15.1%). Thus, we can assume that the phytoplankton community formed in 1994 was “younger” than in 1995 and, hence, its production and the rate of utilization of biogenic elements were higher. It is also impossible to exclude the influence of various other factors, such as, e.g., the specific features of the hydrometeorological situation preceding the survey, the variations of the quality of waters of the river discharge, etc.

The events of penetration of the tongue of transformed river waters were also detected in the late autumn period of the year corresponding to the seasonal increase in the discharge of the River Dnieper (e.g., in October 1996; see Fig. 2.12). In this case, the region of freshening is characterized by the elevated concentrations of chlorophyll A and phosphorus of phosphates and low concentrations of ammonium nitrogen. However, unlike spring, as a result of the intense convective mixing of waters in the autumn–winter period of the year, the freshened regions with elevated contents of biogenic elements and the maxima of the biomass of phytoplankton in the surface layer of the water area are also formed in the regions of deepened discharge of the sewage waters of the cities of Odessa, Il’ichevsk, and Yuzhnyi.



(a) **(b)**

Fig. 2.12. Space distributions of: (a) salinity (‰) and (b) chlorophyll A (mg Chl A/m³) in the surface layer of the Odessa region in the northwest part of the Black Sea (October 1996).

The detailed description and comparative characteristics of the coastal anthropogenic sources of pollution in the investigated water area can be found in [36, 86, 104]. In Table 2.7, we characterize the contributions of each group of anthropogenic sources to the pollution of marine media in the Odessa region. It is easy to see that the "Yuzhnaya" and "Severnaya" stations of biological cleaning are the most powerful identified sources of pollution of the water area. In total, they deliver 38% nitrates, 79% nitrites, 86% ammonium nitrogen, 87% phosphates, and 69% organic substances of the total amount of these substances coming to the marine medium from the coastal anthropogenic sources. At the same time, the contribution of the other analyzed sources of pollution cannot be neglected (Fig. 2.13). Thus, about 13% of the total discharge of organic matter and 83% of the discharge of oil products come with the storm discharge. Note that, unlike the other sources of pollution, this type of discharge occurs with high intensities for short periods of time during the days of heavy showers. Clearly, in these periods, the contribution of storm discharge to the pollution of the coastal zone of Odessa is predominant as compared with the other anthropogenic sources. The discharge of drainage waters is a significant source of nitrate nitrogen (about 18%). The sewage waters of the Odessa Harbor Plant, harbor, and the city of Yuzhnyi give 28% of the total amount of nitrates and almost 10% of the total amount of phosphates.

As a result of functioning of the coastal anthropogenic sources, the maximum concentrations of biogenic substances are observed in the regions of location of the principal sources of pollution, i.e., near the Severnaya and Yuzhnaya stations of biological cleaning, in the Odessa Bay, and at the sites of discharge of the Odessa Harbor Plant and Il'ichevsk Harbor (Fig. 2.14). Significant amounts of oil products penetrate into the water area of the Odessa region with sewage waters of the coastal anthropogenic sources. As a result, the concentrations of these substances may exceed the maximum permissible concentrations (Fig. 2.15).

Table 2.7. Relative Contributions of the Coastal Anthropogenic Sources to the Pollution of the Odessa Region of the Northwest Part of the Black Sea

Anthropogenic sources of pollution	Water flowrate, $10^6 m^3$/yr	Standard parameters of pollution											
		BOD_{tot}		Nitrates		Nitrites		Ammonium		Phosphates		Oil products	
		tons/yr	%	tons N/yr	%	tons N/yr	%	tons N/yr	%	tons P/yr	%	tons/yr	%
"Severnaya" station of biological cleaning	75.70	608.90	31.6	551.00	22.9	12.8	42.6	136.00	38.4	356.00	52.2	4.56	5.4
"Yuzhnaya" station of biological cleaning	52.70	716.70	37.3	376.00	15.7	11.0	36.7	169.00	47.8	238.00	34.9	1.53	1.8
Il'ichevsk Sea Harbor	9.10	52.11	2.7	34.47	1.4	2.89	9.6	19.82	5.6	17.28	2.5	0.39	0.5
Odessa Harbor Plant	8.50	30.50	1.6	664.28	27.6	1.21	4.0	16.10	4.5	66.94	9.8	0.85	1.0
Discharges: Storm	2.90	246.48	12.8	4.21	0.2	1.00	3.3	1.38	0.4	0.37	0.1	69.9	82.7
Drainage	19.45	102.71	5.3	425.90	17.7	0.42	1.4	8.33	2.4	3.07	0.5	3.12	3.7
Industrial	36.21	166.71	8.7	349.30	14.5	0.70	2.4	3.17	0.9	—	—	4.14	4.9
Total	204.56	1924.10	100	2405.16	100	30.02	100	353.80	100	681.66	100	25.29	100

In Table B.4, we present the qualitative compositions of sewage waters coming to the marine media from the Odessa Severnaya and Yuzhnaya stations of biological cleaning, the cities of Il'ichevsk and Yuzhnyi, the Il'ichevsk Sea Harbor, and the Odessa Harbor Plant. The data on the amount of discharged waters from the other anthropogenic sources of pollution and their qualitative composition can be found in the works cited above.

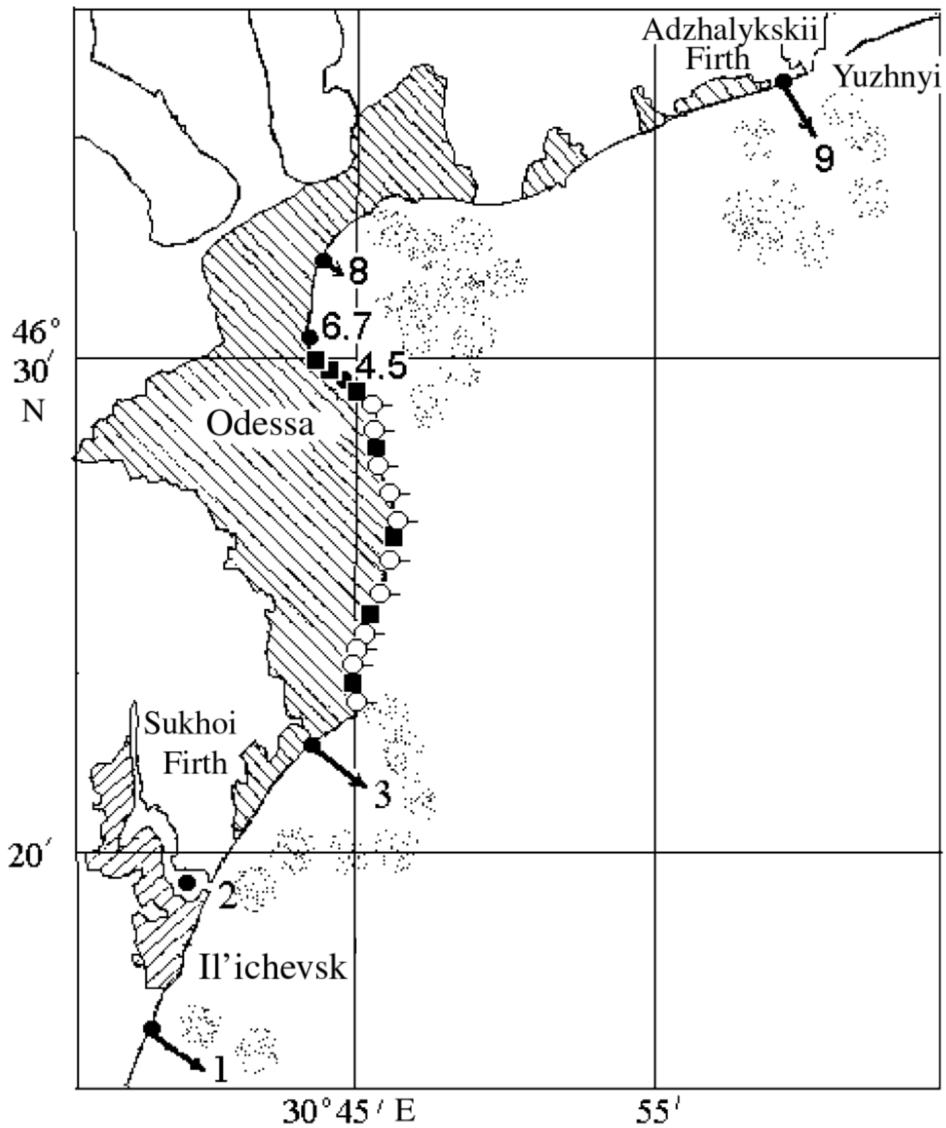
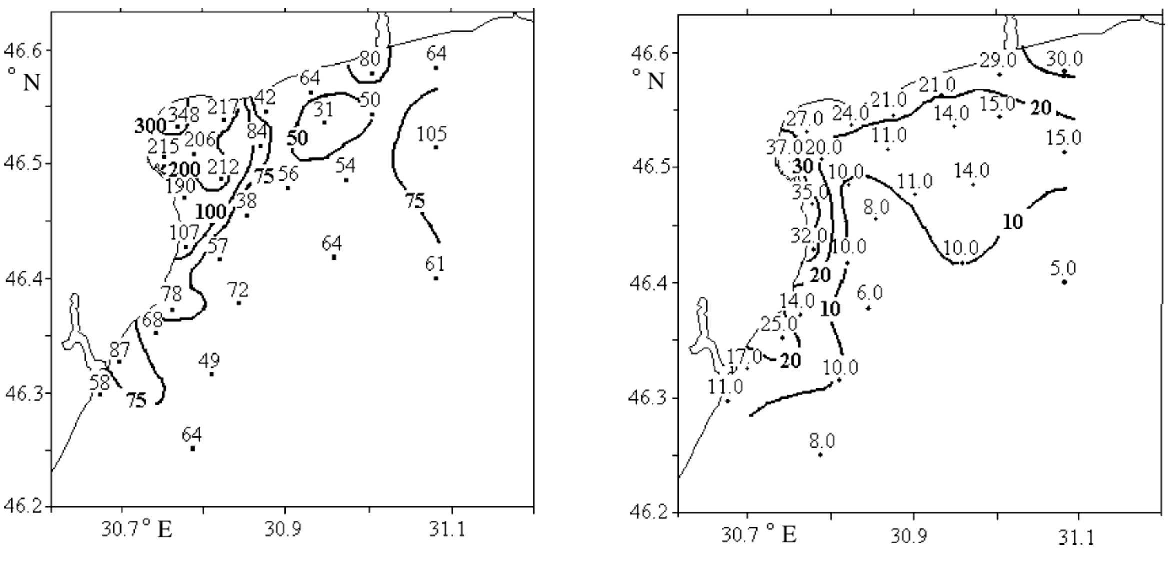


Fig. 2.13. Main sources of pollution of the marine media in the Odessa region of the northwest part of the Black Sea: (1, 2) city of Il'ichevsk and the Il'ichevsk Commercial Sea Harbor, (3) Yuzhnaya Station of biological cleaning, (■) storm discharge, (○) drainage discharge, (4) objects of the Odessa Harbor, (5) "Ukraina" Ship-repairing Yard, (6) Odessa Sugar Company, (7) Odessa Heat-and-Electric Plant, (8) Severnaya Station of biological cleaning, (9) Odessa Harbor Plant.

In the spring-and-summer period of the year, a sharp pycnocline is formed as a result of heating of the surface waters and under the influence of river discharge (in spring) and weakening of the wind activity (in summer). The pycnocline blocks the mass and gas exchange between the surface and deeper layers.



(a) **(b)**

Fig. 2.14. Distributions of ammonium nitrogen (μgN/liter) in May 1998 (a) and phosphorus of phosphates (μgP/liter) in September 1999 (b) in the surface layer of the Odessa region in the northwest part of the Black Sea.

Under these conditions, an especially important role in the supply of the surface photic layer with biogenic elements and, hence, in the stimulation of the process of primary production of organic matter by phytoplankton is played by the littoral wind-induced upwelling of waters observed under the action of offshore winds.

In view of the morphometric features of the analyzed water area in the Odessa region, all winds of the west directions (from north to south) can potentially play the role of offshore winds. However, the lowest wind-induced values of the surge are observed in the presence of the northwest winds whose repeatability in summer is maximum and varies within the range 22–28% [21]. In the presence of the southwest and south winds, the Ekman-type upwelling may develop along the west coast of the water area [8]. The general repeatability of the offshore winds in summer reaches 50%, which enables one to treat coastal upwelling as a phenomenon typical of the investigated region.

The wind surges and coastal upwelling of waters in the Odessa region are described in [33, 94, 102, 106]. In the period of low level of the surge, the thermocline rises to the sea surface in the coastal zone of the sea with a width of about 5 km. In this case, cold and relatively salty transparent abyssal waters enriched with mineral compounds of nitrogen and phosphorus penetrate into the surface photic layer. As a result of this process, the biomass grows in the zone of temperature front characterized by the formation of optimal (over the entire family of the factors of influence) conditions for the synthesis of "new" production.

The fact that upwelling exerts a favorable influence on the productivity of plankton in the Black Sea is confirmed by the experimental results presented in [43].

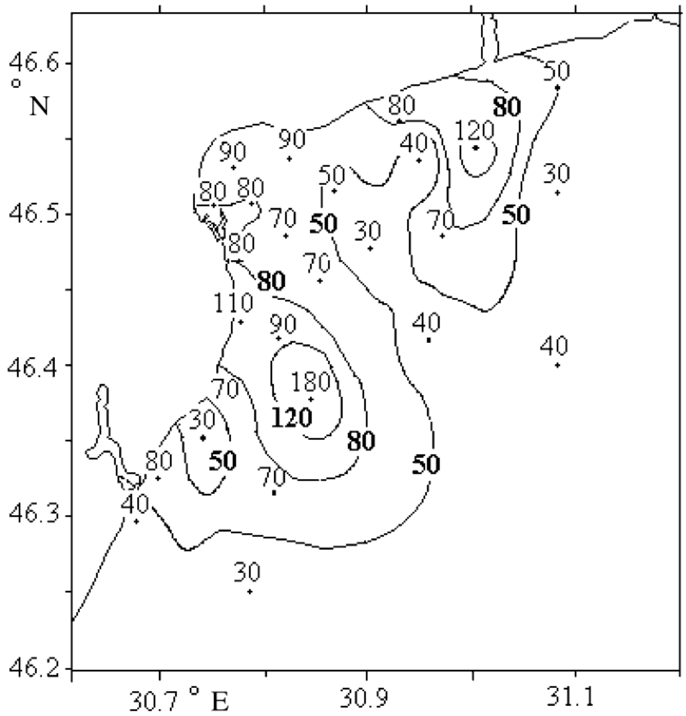


Fig. 2.15. Contents of the oil products (μg/liter) in waters of the surface layer of the Odessa region in May 1998.

In the course of monitoring carried out by the Odessa Branch of the Institute of Biology of Southern Seas, extensive phenomena of low-level surges were recorded in the surveys of August 1988, 1990, and 1994 [33, 102, 106]. Weak local traces of the coastal upwelling were detected in August 1992, 1995, and 1998.

In Fig. 2.16, we present the situation recorded in the presence of weakly developed but extensive upwelling in August 1994. We see that the maximum values of primary production of phytoplankton, content of chlorophyll A, and the biomass of phytoplankton correspond to a belt of surface waters with lower temperatures and elevated salinities stretched along the west coast of the analyzed region. Note that the signs of upwelling were present in the space distributions of biogenic elements (in the form of elevated concentrations of these elements). However, they were not so clear as in the field of phytoplankton. This is not surprising in view of the high rates of utilization of mineral compounds of biogenic elements by phytoplankton in the process of photosynthesis in summer and the spatial inhomogeneity of their penetration into the surface layer caused by the presence of near-bottom discharges of industrial and municipal sewage waters near Cape Bol'shoi Fontan (Yuzhnaya station of biological cleaning in Odessa) and in the Sukhoi Firth (Il'ichevsk).

Since the early 1970s, the hypoxic-anoxic phenomena responsible for the mass death of organisms living in bottom layer and benthic organisms have been systematically recorded in the northwest part of the Black Sea in summer (July–September). It is customary to believe that the redundant penetration of biogenic substances in marine media as a result of the human economic activity is the main cause of hypoxia.

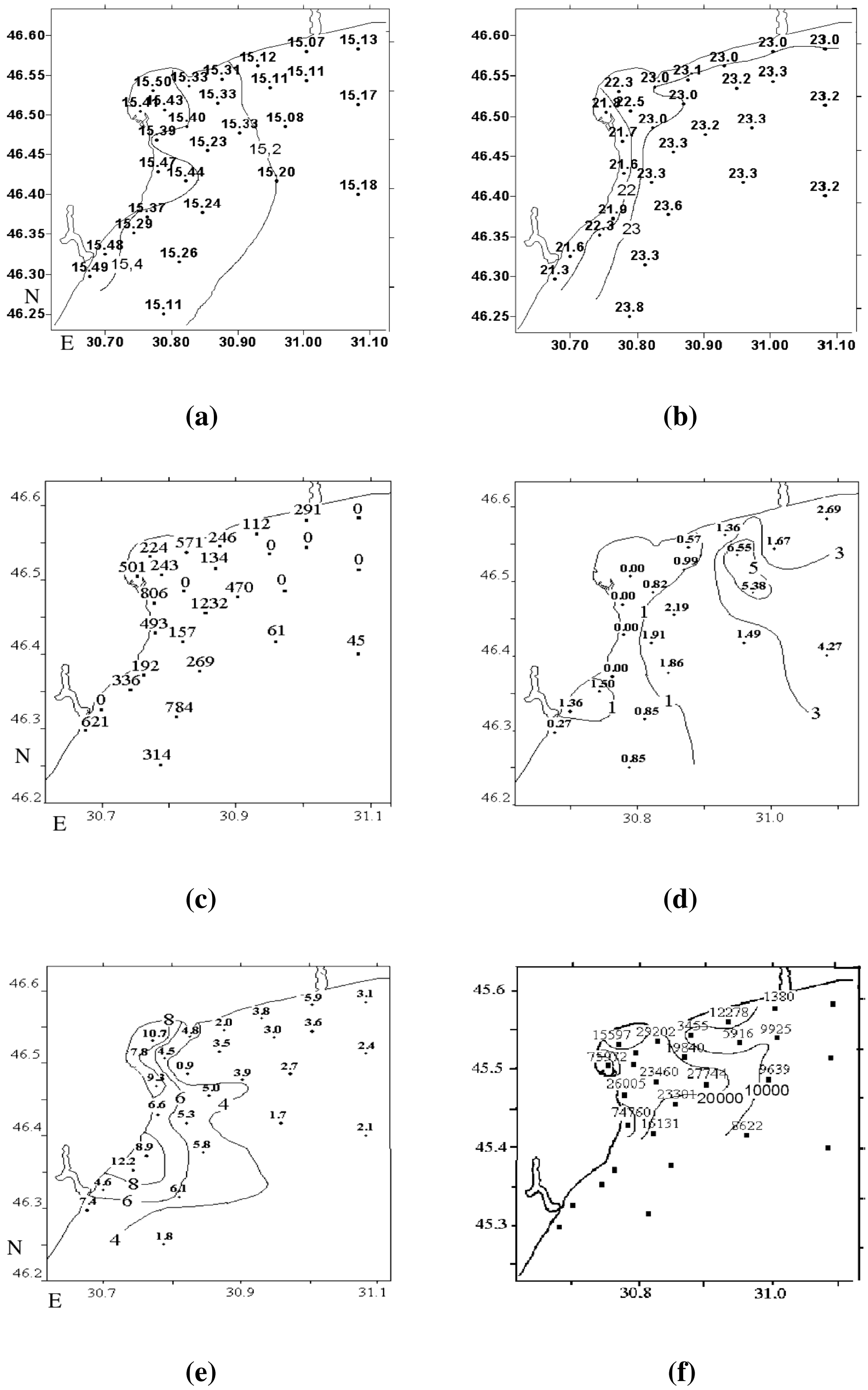


Fig. 2.16. Space distributions of various parameters over the surface layer of the Odessa region in the northwest part of the Black Sea in August 1994: (a) salinity of water (‰), (b) temperature of water (°C), (c) net production of phytoplankton [mgC/(m^3day)}, (e) chlorophyll A, (mg Chl A/m^3), (f) biomass of phytoplankton (mg/m^3), and (d) the concentration of dissolved oxygen (mg/liter) in the bottom layer.

Table 2.8. Hydrochemical Characteristics of the River Discharge Affecting the Quality of Waters in the Dnieper–Bug and Odessa regions of the Northwest Part of the Black Sea [19, 30]

River	NH_4^+, mgN/liter	NO_3^-, mgN/liter	PO_4^{3-}, mgP/liter	O_2, mg/liter	BOD_5, mg/liter	Oxidizability by $KMnO_4$, mg/liter
Dnieper	0.44	1.54	0.12	7–13	2.94	9–14
Yuzhnyi Bug	0.56	1.54	0.074	8–13	2.46	7–13
Dniester	0.29	0.18	0.14	13	2.98	—

Note that rivers are the main suppliers of these substances. The hydrochemical characteristics of the discharges of Dnieper, Yuzhnyi Bug, and Dniester Rivers are presented in Table 2.8 (according to the data of [19, 30]).

As shown in [102], the development of upwelling in the coastal zone of the Odessa region is correlated with the formation of hypoxia in the bottom layer over the continental slope. In most cases, the sites of hypoxia in the bottom layer of the coastal zone correspond to the sites of minimum temperature of water in the surface layer (Fig. 2.17). Moreover, the phenomenon of hypoxia is absent in the bottom layer of the deeper open-sea part of the water area. The most reliable explanation of this correlation can be given by using the results presented in [77], where, on the basis of the data of vertical sounding of the oxygen content of waters in the northwest part of the Black Sea in the summer–autumn period of the year, it is shown that the formation and initial development of the hypoxic-anoxic conditions are observed not in the bottom layer (as was assumed earlier) but in an intermediate layer on the lower boundary of the pycnocline. In the presence of long-term or strong offshore winds, the lens of hypoxic waters under the pycnocline migrates toward the coast and rises to the surface over the continental slope. As a result, the phenomenon of hypoxia is detected in the bottom layer of the coastal zone but not in the abyssal open-sea part of the water area.

However, it is necessary to take into account the fact that the low-level surges promote the inflow of biogenic substances from the bottom layer and, hence, stimulate the production of organic matter in the coastal zone. At the end of the low-level surges, this matter moves to the coast and, as a result of gravitational sedimentation, appears in deeper layers, where dissolved oxygen is used for its oxidation. Thus, the low-level surges can directly initiate the development of hypoxia in the bottom layer of the coastal zone.

The phenomenon of coastal upwelling can also develop in spring. Thus, the belt of waters with lower temperatures and elevated salinities detected in the survey carried out in May 1994 (Figs. 2.10a, b) in the central part of the analyzed water area is a result of the Ekman-type wind-induced upwelling initiated by the strong south wind recorded for several days during the period of the survey.

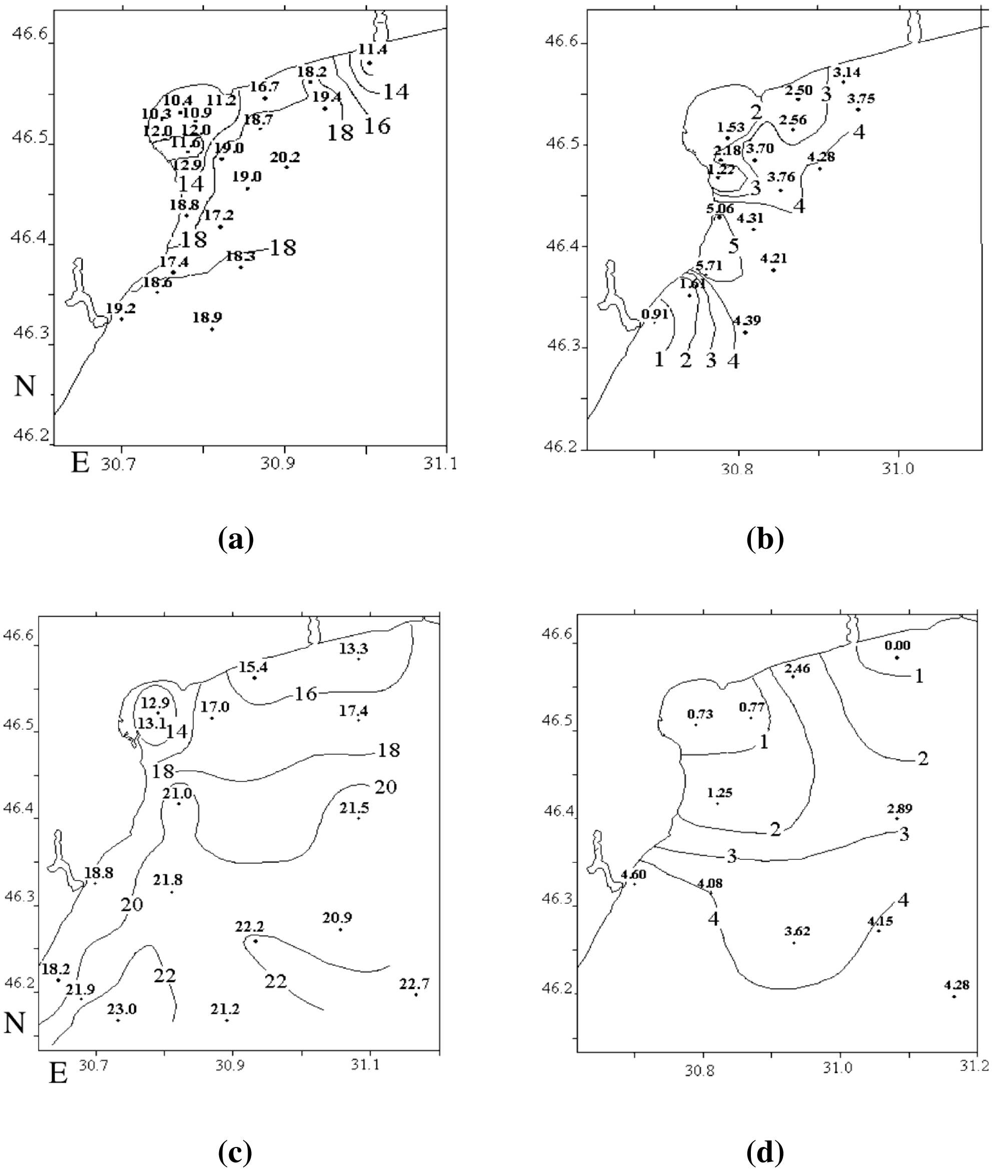


Fig. 2.17. Space distributions of the: (a, c) temperature of water (°C) in the surface layer, (b, d) content of dissolved oxygen (mg/liter) in the bottom layer of the Odessa region in the northwest part of the Black Sea in August 1988 (a, b) and August 1990 (c, d).

As follows from Fig. 2.10f, the maximum biomass of phytoplankton is observed in the zone of hydrofront separating relatively warm freshened waters with elevated concentrations of phosphates and cold more transparent waters of the zone of upwelling enriched with mineral nitrogen.

In Table 2.9, we present the average values and ranges of the basic hydrochemical parameters of the analyzed water area for different hydrological seasons computed according to the data of ecological monitoring carried out by the Odessa Branch of the Institute of Biology of Southern Seas in 1988–1999 for the surface and bottom layers.

To study the role played by the local anthropogenic sources of pollution, the statistical characteristics were determined separately for the coastal stations and the stations made in the open part of water area. The stations located directly near the coastline were regarded as coastal (Fig. 2.18).

Table 2.9. Average Values (Numerators) and Ranges (Denominators) of the Basic Hydrochemical Characteristics of Eutrophication of the Coastal and Open-Sea Zones of the Odessa Region in the Northwest Part of the Black Sea

Season	Zone	Layer	pH	O_2, mg/liter	BOD_5, mg/liter	NH_4, μgN/liter	NO_2, μgN/liter	NO_3, μgN/liter	N_{org}, μgN/liter	PO_4, μgP/liter	P_{org}, μgP/liter
Spring	Coastal	surface	8.48 / 8.15-8.83	10.4 / 7.6-12.3	2.13 / 0-8.0	83.6 / 8-550	1.3 / 0-12.2	21.0 / 0-108	578.3 / 75-1624	9.0 / 0-25	21.8 / 5-60
		bottom	8.27 / 7.9-8.69	9.5 / 3.8-12.5	1.33 / 0-3.4	93.2 / 0-470	2.9 / 0-11.7	28.4 / 3-74	628.3 / 78-3670	13.8 / 2.7-44	16.6 / 0-44
	Open-Sea	surface	8.48 / 8.21-8.82	10.3 / 8.6-12.2	1.75 / 0-6.7	69.2 / 13-320	1.4 / 0-11.5	28.1 / 0-141	594.7 / 104-3615	7.1 / 0-20	19.3 / 7-40
		bottom	8.28 / 8.02-8.51	10.0 / 5.4-14.4	1.34 / 0-3.1	77.6 / 0-276	3.9 / 0-16.7	33.8 / 0-93	640.8 / 152-3741	9.7 / 0-43	15.8 / 0-55
Summer	Coastal	surface	8.39 / 7.8-8.9	8.3 / 2.6-11.9	2.46 / 0.3-8.5	164.3 / 12-1600	2.0 / 0-19.0	51.7 / 0-1147	668.2 / 32-2610	17.8 / 0-382	40.9 / 1-262
		bottom	8.01 / 7.56-8.77	4.2 / 0-9.8	1.65 / 0-5.1	189.5 / 15-735	5.9 / 0-33.0	50.4 / 0-318	648.7 / 0.2-2700	29.5 / 0-160	40.0 / 0-210
	Open-Sea	surface	8.49 / 8.04-8.91	8.8 / 7.4-11.1	2.25 / 0.5-5.5	89.6 / 12-400	1.8 / 0-19.0	53.5 / 0-210	701.5 / 9-2733	8.9 / 0-43	26.6 / 3-126
		bottom	8.03 / 7.43-8.74	4.6 / 0.8-9.5	1.56 / 0-5.1	114.1 / 10-420	6.6 / 0-28.0	81.1 / 1-191	670.2 / 6-2131	21.4 / 5-50	23.9 / 0-123

Season	Zone	Layer	pH	O_2, mg/liter	BOD_5, mg/liter	NH_4, µgN/liter	NO_2, µgN/liter	NO_3, µgN/liter	N_{org}, µgN/liter	PO_4, µgP/liter	P_{org}, µgP/liter
Autumn	Coastal	surface	8.31 / 8.0-8.50	10.6 / 7.4-14.0	1.64 / 0.2-4.0	109.9 / 9-870	7.2 / 0.5-15.2	73.4 / 2-163	729.0 / 45-2104	27.4 / 10-68	21.4 / 6-66
		bottom	8.26 / 8.0-8.40	9.5 / 6.7-12.2	1.05 / 0-2.8	92.9 / 10-375	6.8 / 1.9-14.1	90.9 / 6-946	720.2 / 214-1665	24.4 / 5-42	18.7 / 0-50
	Open-Sea	surface	8.32 / 7.45-8.55	11.0 / 9.2-13.8	1.92 / 0.6-6.9	95.1 / 9-700	3.8 / 0.5-9.4	41.3 / 2-114	690.8 / 76-1899	20.0 / 0-38	21.7 / 0-48
		bottom	8.26 / 7.16-8.45	9.7 / 6.6-12.4	1.62 / 0-7.5	86.6 / 10-320	4.1 / 0.3-9.2	36.6 / 8-158	668.0 / 43-3124	18.6 / 0-40	16.3 / 0-30

As follows from the analysis of the seasonal average values of hydrochemical characteristics presented in Table 2.9, the minimum concentrations of phosphates in the photic layer (7–9 µgP/liter) are observed in spring and summer (in the surface layer of the open-sea part of the water area). The concentration of ammonium is minimum in spring (70–80 µgN/liter) and reaches its maximum values in the coastal zone of the sea in summer (up to 164 µgN/liter). The minimum concentrations of nitrites and nitrates are observed in spring (20– 30 µgN/liter) and the maximum concentrations are attained in the coastal zone of the sea in autumn (80–90 µgN/liter). For the whole year, the concentration of ammonium nitrogen is higher than the concentration of nitrates.

In the spring–summer period when the utilization of biogenic elements by phytoplankton in the course of photosynthesis in the photic layer is maximum and the mass exchange between the surface and bottom layers is hampered by the presence of pycnocline, the difference between the seasonal average concentrations of ammonium nitrogen in the indicated layers does not exceed 15% in the coastal zone and 27% in the open-sea part of the water area. At the same time, the difference between the concentrations of mineral phosphorus can be as high as 65 and 140%, respectively.

The development of hypoxia in the bottom layer in summer promotes the intensification of the fluxes of ammonium and phosphates from the bottom sediments, deceleration of the process of nitrification, and decrease in the content of nitrates as a result of denitrification. Hence, the maximum concentrations of phosphates and ammonium are detected in the bottom layer of the water area in summer.

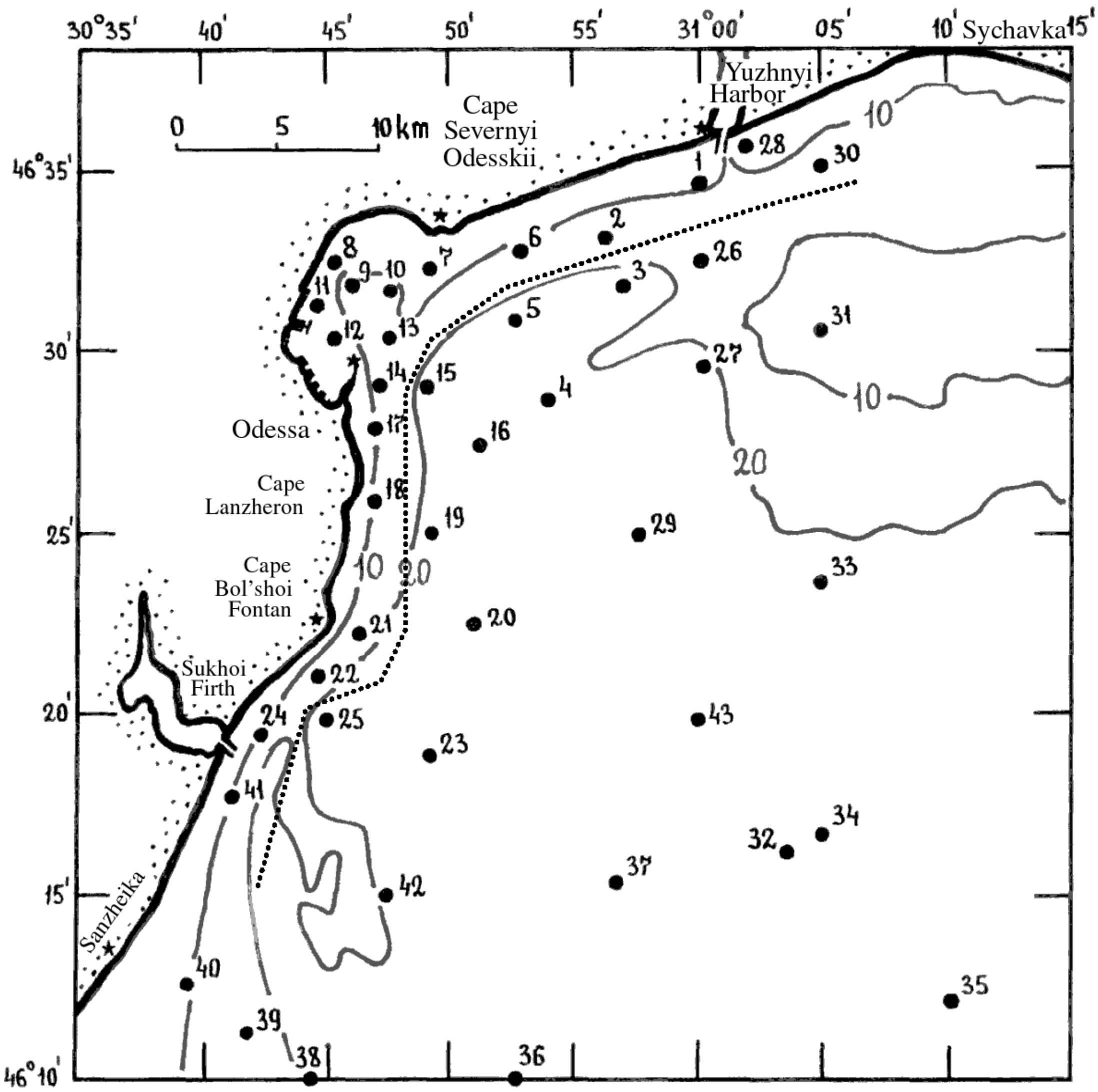


Fig. 2.18. Schematic map of location of the stations of ecological monitoring of the Odessa Branch of the Institute of Biology of Southern Seas in the Odessa region of the northwest part of the Black Sea. The isobaths are shown by solid lines. The dotted line separates the stations conditionally regarded as coastal.

The comparison of the average concentrations of mineral compounds of nitrogen and phosphorus in the surface layer of the Odessa region (Table 2.9) with the data of literature sources on the typical values of semisaturation constants of the growth rate of phytoplankton with respect to these biogenic elements (see Subsection 5.1) enables us to assume that the photosynthesis of organic matter in spring and summer can be limited by the lack of mineral phosphorus rather than by the lack of nitrogen.

The concentrations of organic compounds of nitrogen and phosphorus in spring and summer significantly exceed the concentrations of their mineral compounds (on the average, they are 2–3 times higher for phosphorus and 3–6 times for nitrogen higher). In autumn, the ratio of the concentrations of organic and mineral compounds of phosphorus becomes equal to 1 or even lower. At the same time, for nitrogen, this ratio remains constant. The maximum concentrations of organic nitrogen (730 μg N/liter) and phosphorus (27 μg P/liter) are detected in autumn in the coastal zone of the sea.

The annual average value of the ratio of the concentrations of mineral compounds of nitrogen and phosphorus N:P in water is equal to 10 : 1. At the same time, for the organic matter it is equal to 30 : 1. This ratio may change to the side of nitrogen for the inert organic matter under the action of the following two factors: the higher rate of mineralization of organic phosphorus as compared with organic nitrogen and the inflow of organic nitrogen from the anthropogenic sources and rivers in larger amounts than in the case of organic phosphorus.

In general, in all seasons of the year, the average concentrations of ammonium nitrogen and phosphates in the coastal zone are higher than the concentrations typical of the open-sea part of the investigated water area. The indicated difference attains its maximum values in the surface layer in summer and can be as large as 80% for ammonium and 100% for phosphates. In spring and summer, the littoral waters contain less nitrates and nitrites than the waters of the open part of water area. However, in autumn, their concentration in the coastal zone becomes higher than in the open-sea part of water area (by 78 and 148% in the surface and bottom layers, respectively).

The elevated concentrations of phosphates and ammonium in the coastal zone of the Odessa region can be explained by the influence of the discharge of municipal, storm, drainage, and industrial waters of Odessa, Yuzhnyi, and Il'ichevsk and their harbors (Fig. 2.13), as well as by the already indicated specific features of hydrological conditions formed in the analyzed water area. Among these specific features, we can especially mention the inflow of large amounts of allochthonous organic matter and biogenic substances along the north coast in spring with the tongue of freshened waters from the Dnieper–Bug Firth (Table 2.8) and the penetration of biogenic substances from the bottom layer into the photic layer as a result of the coastal wind upwelling in late spring and summer.

2.2.2. Tuzla Firths

The Tuzla group of firths and lagoons located in the central part of the Danube–Dniester interfluve can be described as a group of shallow-water periodically open basins (Fig. 2.19). This group includes three main firths: Shagany, Alibei, and Burnas, and a family of smaller lagoons (Fig. A.4). The basin is separated from the neighboring water area of the sea by a bay-barrier spit, which can be partially washed away in spring and autumn during the periods of strong storms. Thus, as indicated in [85], about 15 breaks were formed in a 25-km section of the spit after the storm in March 1970. Furthermore, artificial periodically opened channels (whose number may vary) are made in the bay-barrier spit for the needs fishery. Thus, a channel was made for the needs of gray-mullet breeding in the southwest part of the Shagany Firth more than 100 yr ago. Three channels were made in the bay-barrier spit after the Second World War [85] and two in 1995 [91]. These channels are opened only in spring (to give the way for the fries of gray mullet coming from the sea into the basin) and in autumn (to catch the fish going from the firths into the sea directly in the channels).

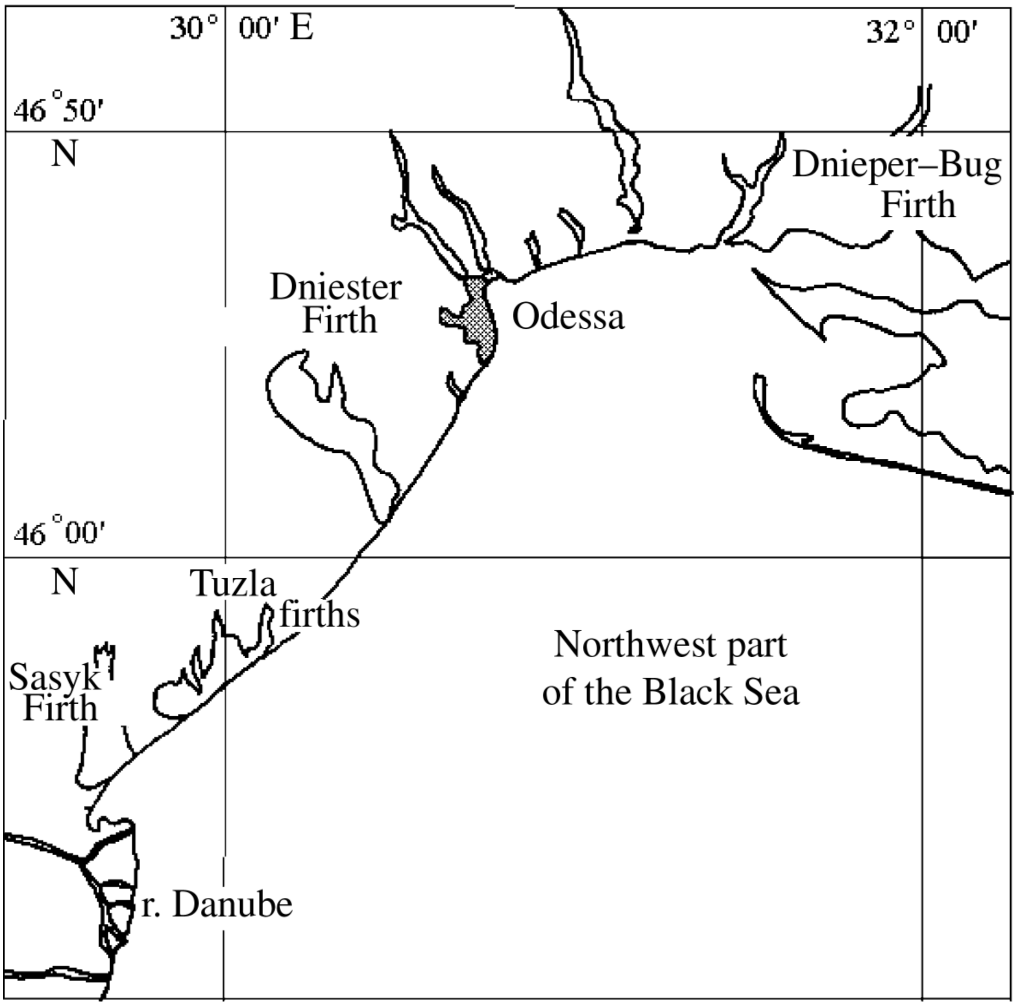


Fig. 2.19. Schematic map of the Tuzla firths.

Among the main natural factors responsible for the formation of the water and saline balance in the Tuzla group of firths, we can mention the surface (slope and river) discharge, precipitation, evaporation, and water exchange with the open sea through the artificial channels and natural breaks. The role of the inflow of ground waters and filtration of seawater through the bay-barrier spit is small as compared with the water exchange through the breaks and channels [85].

Since the freshwater balance of the Tuzla group of firths is negative (the intensity of evaporation is several times higher than the intensity of precipitation), the salinity of waters is determined mainly by the water exchange with the sea through the channels. In the summer period of the year when the water exchange with the sea is absent and evaporation is quite intense, the salinity of waters in the firth increases from 15‰ in spring to 34‰ in summer. As for the average salinity of waters, the firths can be arranged as follows: Burnas (26‰), Alibei (28‰), and Shagany (29‰). Moreover, the ranges of variability of the level of salinity constitute 12–32‰ for Burnas, 16–31‰ for Alibei, and 18–35‰ for Shagany [85]. The minimum levels of salinity are detected in spring and correspond to the maximum filling of the firths due to the penetration of waters from the sea. The maximum levels of salinity are attained at the end of summer when the height of water in the basin is minimum due to evaporation. In general, the level of salinity of waters in the firth is always higher than in the neighboring water area of the sea. Indeed, in spring, it is higher by several parts per thousand and, in summer, twice higher. Thus, the exchange of waters between the firth and the sea results in a relative "freshening" of waters in the firth and is favorable for the gray-mullet fishery.

According to [47], in the absence of water exchange with the sea, the firths rapidly become shallow and a period of 3–4 yr is sufficient for their complete drying. It is well known that, in the 19th century, the salinity of waters in the firths reached 200‰, and this region was used for the commercial extraction of salt. As a result of the catastrophic drop of the level of water in 1868–1869, the Tuzla firths turned into hyperhaline marshy saline soils. In summer 1915, the salinity of their waters was equal to 100–140‰ and only after the appearance of stable periodic artificial communication of the firths with the sea, the level of salinity decreased to 20–40‰.

A detailed hydrobiological characteristic of the Tuzla firths from the viewpoint of fishery can be found in [91]. It is indicated that, despite fairly high food resources for fish, the actual fish productivity of the firths is low. This is explained by the specific natural characteristics of the firths (shallowness, isolated character, high levels of salinity, winter overcooling, and summer overheating of water to 27–30°C) unfavorable for the reproduction of the most species of fishes encountered in the neighboring water area of the sea.

The principal direction of the economic utilization of the Tuzla group of firths is connected with the controlled pasture fish (gray mullet and silversides) breeding based on the use of the specific feature of the behavior of Black-Sea gray mullet and silversides visiting the firths in spring for fattening and migrating to the sea in autumn. However, for the last years, the catches of gray mullet and silversides have become much lower due to the decrease in their number in the neighboring water area of the sea as a result of the general deterioration of the ecological situation [91]. Hence, the problem of development of specific scientifically justified recommendations aimed at the rational and complex utilization of natural resources of the analyzed group of firths and elevation of their fish productivity seems to be quite urgent. Clearly, the solution of this problem is connected with the rational management of water exchange between the firths and the sea. The efficiency of various administrative and engineering decisions aimed at getting the required parameters of the quality of waters in the firths can be estimated by the method of mathematical simulation.

Conclusions

The marine water areas of the tropical and middle latitudes studied in our book have serious ecological problems connected with the anthropogenic intrusion and loads.

Thus, about 60 and 40% of crude municipal sewage waters of the city of Cartagena are discharged into the Ciénaga de Tesca shallow-water tropical lagoon and the deep-water Cartagena Bay (with shallow-water sea straits), respectively. In addition, the industrial sewage waters of enterprises located in the industrial zone of Cartagena and polluted waters of the Dique Channel connecting the bay with the Magdalena River also penetrate into the Cartagena Bay. As a result, even according to the standards used for the surface waters of dry land, the quality of waters in the Ciénaga de Tesca Lagoon corresponds to the state of highly polluted (hypertrophic and polysaprobic) basins. Furthermore, the Cartagena Bay is characterized by a high level of pollution of waters with pathogenic bacteria and periodic development of hypoxia in its bottom layer.

In the shallow-water Ciénaga-Grande-de-Santa-Marta Firth, due to the absence of the ecological substantiation of engineering decisions, the process of natural water exchange with the sea was violated, which led to the mass death of unique mangrove thickets. The increase in the inflow of fresh waters from the Magdalena River through the system of artificial channels solved the problem of strong salinization of small sea lakes but did not lead to the restoration of perennial mangrove thickets and caused new problems connected with the eutrophication of the basin, periodic death of new species of mangroves as a result of flooding, and deterioration of the conditions of functioning of the marine economy.

In the analyzed tropical marine ecosystems, the primary production is limited not by the biogenic elements but by the low transparency of water. The shallow-water basins are characterized by very high values of biochemical oxygen demand and the concentrations of organic matter. The current state of these ecosystems is very sensitive to climatic oscillations connected with the development of the phenomenon of El Niño.

The quality of waters in the Odessa zone of the Dnieper–Bug estuary region in the northwest part of the Black Sea is determined by the inflow of biogenic and toxic substances with the discharge of the Dnieper, Yuzhnyi Bug, and Dniester Rivers and as a result of functioning of the anthropogenic sources of pollution in the coastal zone. The concentrations of some kinds of pollutants (e.g., oil products, BOD, and pathogenic microflora) in waters of the Odessa region can exceed the maximum permissible concentrations. In this region, the waters are strongly eutrophied and characterized by the development of the phenomenon of hypoxia under the pycnocline in summer. The primary production of phytoplankton in spring and summer can be limited by the insufficient amount of mineral phosphorus.

The current space distributions and variability of the hydrochemical and hydrobiological characteristics of waters are strongly affected by the following hydrological phenomena typical of this region: penetration of a tongue of freshened waters from the Dnieper–Bug Firth in spring and coastal wind-induced upwelling in the spring–summer period of the year. The development of these phenomena is accompanied by the penetration of additional amounts of biogenic mineral and organic substances into the Odessa region and, hence, promotes the intensification of the process of eutrophication of its waters.

The tongue of transformed river waters coming into the analyzed region from the Dnieper–Bug Firth in spring is characterized by the elevated contents of chlorophyll A and the biomass of phytoplankton because high concentrations of biogenic substances in river waters promote the primary production of organic matter by phytoplankton. Under the action of the gravitational forces, this organic matter suffers sedimentation and is deposited in bottom sediments, thus increasing the probability of development of hypoxia in the bottom layer of this region in summer.

On the one hand, the systematic low-level surge phenomena in the coastal zone of the sea in summer promote the enrichment of the photic layer with biogenic substances and, hence, stimulate the primary production of organic matter which, as a final result, comes into the layers located below the pycnocline due to gravitational sedimentation and oxidizes, thus inducing the development of hypoxia. On the other hand, the low-level surges are accompanied by the penetration of hypoxic waters of the intermediate layer into the most productive coastal zone of the sea, which leads to the recurrent development of the hypoxic-anoxic conditions in this zone and death of the hydrobionts.

Hence, in the years when the wind conditions formed near the Odessa coast are favorable for the frequent intense long-term freshening of waters in spring and the development of coastal upwelling in summer, the probability and intensity of development of the hypoxic phenomena in the bottom layer of the investigated region increase.

For the Tuzla group of firths, the main problem is connected with their low fish productivity observed despite the presence of fairly rich food resources and explained by the specific features of their morphology and hydrological conditions. In the absence of artificial water exchange with the sea, these firths may suffer both strong shallowing and increase in the level of salinity of their waters.

Thus, all analyzed water objects and water areas of the shelf zone of the sea require the development of scientifically substantiated recommendations and prognostic estimations of the efficiency of measures aimed at the stabilization and improvement of their ecological state. To solve this problem, we use the methods of numerical mathematical simulation of the dynamics and quality of waters in the sea.

3. HYDRODYNAMIC BLOCK OF THE MODEL OF QUALITY OF WATERS IN SHELF ECOSYSTEMS

The shelf zone of the sea is characterized by its own specific features distinguishing it from the open part of the ocean. In this connection, we should mention, first of all, the ageostrophic character of motions and strong influence of the morphometric features of the analyzed water area (bottom topography, configuration and irregularities of the coastline, and the presence of gulfs, bays, and firths whose water exchange with the open sea is restricted) on the dynamics of waters.

In shallow-water and (to a significant extent) isolated parts of the shelf (firths and lagoons), the role of the main driving force responsible for the motion of waters is played by the wind stresses acting upon the sea surface. Owing to the formation of turbulent stresses in the liquid, the influence of the wind can be observed at fairly large distances from the sea surface. The wind currents suffer the influence of the bottom detected, first, in the interaction of the (bottom and surface) turbulent boundary layers and, second, in the formation of slopes of the sea surface caused by the presence of the coasts and inhomogeneities of the bottom topography leading to the development of gradient currents.

In partially isolated regions of the sea (bays and estuaries), the role of the sources of motion is also played by the momentum transfer through the liquid boundary and the oscillations of the sea level caused both by the surges and tidal phenomena and penetration of the water masses with river discharge. The presence of "liquid boundary" is responsible for the interaction of the circulation of waters in the analyzed water area with large-scale circulation.

Further, an important role in the dynamics of waters in the shelf zones is played by the following stratifying factors: freshwater river discharge and thermal inhomogeneities caused by the spatial variations of the intensity of absorption of solar radiation in the water column, heat exchange between water and air, wind-induce turbulent mixing of the surface waters, and coastal upwelling.

The thermohaline structure and the dynamics of waters become especially complicated in the estuary zones of the shelf characterized by the sharpening of the space gradients of temperature and salinity of waters and the intensification of currents with thermohaline, gradient, and wind components of the same order of significance. The process of sharpening of the horizontal gradients of water temperature in the estuary zones is also promoted by the inflow of large amounts of suspended organic and inorganic particles with river discharge. These particles strongly affect the transparency of water and, hence, the intensity of absorption of solar radiation in the surface layer.

The estuary parts of the shelf zone are of especial interest for the solution of various nature-preservation problems because rivers play the role of the most powerful sources of pollution of marine media. The water catchment area of the major part of rivers is a zone of intense human economic activity. Therefore, river waters accumulate significant amounts of polluting substances of the anthropogenic origin coming from the water catchment areas of the rivers.

In the analysis of the influence of rivers on the quality of waters and dynamics of the components of marine ecosystems, it is necessary to be able to determine both the degree and boundaries of this influence and the trajectories of transfer of pollutants with various physical and chemical properties. For the correct solution of this problem, the delta of a river and the neighboring part of the sea should be regarded as a single system with interdependent parts. Thus, the tidal oscillations of the sea level and/or surges affect the flow rate of the rivers in the mouth section and, hence, the transfer of pollutants contained in the river waters. Furthermore, it is often necessary to compute the redistribution of discharge between numerous branches of the river delta depending on the hydrometeorological conditions in the estuary zone.

Numerous bays and firths connected with the open sea by narrow straits are often used as good natural shelters for ships. This explains the intense development of cities-ports on the coasts of these basins whose economic activities and municipal sewage waters create powerful anthropogenic loads upon the marine ecosystem deteriorating the quality of its waters. The self-cleaning ability of the ecosystems of these basins is much lower than in the open water areas due to the limited water exchange with the sea. Therefore, the possibility of correct evaluation of water exchange through the narrow straits (or channels) becomes especially urgent for the regulation of anthropogenic loads upon the marine ecosystems of closed basins [52, 54].

Hence, the mathematical models of the dynamics of waters in the shelf zone of the sea must be able to realize the following tasks:

— describe the wind (drift and compensation), density, tidal, and discharge currents in the domains with significant drops of depth and sharp temperature and salinity gradients, the evolution of the seasonal thermocline, and the variability of the space structure of halocline in the estuary regions;

— perform numerical calculations not only in the estuary regions of the sea but also directly in the river mouths;

— correctly compute the existing water exchange through the narrow straits and/or channels.

All mentioned requirements are met by the hydrothermodynamic model in the formulation and numerical realization proposed in [138, 139] whose initial version was called MECCA (Model for Estuarine and Coastal Circulation Assessment). In the form of the hydrodynamic block, this model serves as a basis for the development of a model of the quality of waters in the shelf marine ecosystems subjected to the influence of river discharge and the loads of anthropogenic sources of pollution located in the coastal zone of urbanized territories. The structure of this model agrees with the structure of the two well-known models proposed in [122, 156].

In the last section of the present chapter, we give the results of adaptation of the hydrothermodynamic model to the conditions of the Dnieper–Bug estuary region in the northwest part of the Black Sea [51] demonstrating the possibility of application of this model to the description of hydrodynamic processes and the hydrology of waters in the estuary zones of the sea shelf at middle latitudes characterized by the well-pronounced seasonal variability of the thermohaline structure of waters.

3.1. Mathematical Structure of the Three-Dimensional Nonstationary Hydrodynamic Model of Formation of the Thermohaline Structure and Circulation of Waters in the Shelf Zones of the Sea

The proposed model is based on the complete system of hydrothermodynamic equations in the Boussinesq approximation and the approximations of incompressibility and hydrostatics. The system includes the equations of motion for the horizontal components of the vector of current velocity, the equations of hydrostatic approximation, the continuity equation, the equation of state, and the equations of conservation of heat and salt. Prior to the analysis of these equations, we introduce the following notation: The partial derivatives of a quantity F are denoted by the subscripts written according to the following rules:

$$\frac{\partial F}{\partial t} = F_t, \qquad \frac{\partial F}{\partial x} = F_x, \qquad \text{and} \qquad \frac{\partial^2 F}{\partial x \partial z} = F_{xz}.$$

The dimensionless vertical coordinate used instead of z is defined as follows:

$$\sigma = \frac{z - h}{h + d},$$

where h is the deviation of sea level from its nondisturbed (average) position and d is the depth of the sea for the nondisturbed level. Thus, on the sea surface, we have $\sigma = 0$ and, at the bottom, $\sigma = -1$.

To specify the location of a quantity on the computational grid in the space, we also use the corresponding subscripts written in the form

$$F(x, y, \sigma) = F_{m,n,l}.$$

By ΔL and $\Delta\sigma$ we denote the horizontal and vertical sizes of a computational cell, respectively. The time steps of the barotropic and baroclinic components of motion are denoted by Δt and ΔT, respectively, where $\Delta t \leq \Delta T$.

In the right-hand Cartesian coordinates, the equations of motion take the following form in the Boussinesq approximation:

$$u_t + \beta_a\{(uu)_x + (uv)_y + (uw)_z\}$$

$$= -\alpha_0 P_x + fv + (2A_h u_x)_x + (A_h[v_x + u_y])_y + (A_v u_z)_z, \quad (3.1)$$

$$v_t + \beta_a\{(vu)_x + (vv)_y + (vw)_z\}$$

$$= -\alpha_0 P_y - fu + (2A_h v_y)_y + (A_h[u_y + v_x])_x + (A_v u_z)_z, \quad (3.2)$$

where u, v, and w are the components of the vector of current velocity $\vec{v}$ in the directions of the x-, y-, and z-axes, respectively, t is time, P is pressure, $\alpha_0 = 1.0$ liter/kg is the constant specific volume of water, ρ is the density of water, f is the Coriolis parameter, A_h and A_v are, respectively, the horizontal and vertical turbulence coefficients, and β_a is a control factor (equal to 0 or 1 and used to switch on or off the terms of advective acceleration).

As the third equation of motion, we use the condition of hydrostatic approximation

$$P_z = -g\rho, \quad (3.3)$$

where $g = 9.81\ \text{m}^2/\text{sec}$ is the gravitational acceleration.

The continuity equation expresses the law of conservation of mass and is written in the form that does not contain acoustic waves:

$$u_x + v_y + w_z = 0. \quad (3.4)$$

The equation of state has the following general form:

$$\rho = \rho_0[1 + F_\rho(T, S)], \quad (3.5)$$

where ρ_0 is the constant density $(\alpha_0 = 1/\rho_0)$ and T and S are, respectively, the temperature and salinity of water. The equations of conservation of heat and salt take the form

$$S_t + (uS - D_h S_x)_x + (vS - D_h S_y)_y + (wS - D_v S_z)_z = 0, \quad (3.6)$$

$$T_t + (uT - D_h T_x)_x + (vT - D_h T_y)_y + (wT - D_v T_z)_z = R, \quad (3.7)$$

where D_h and D_v are the coefficients of horizontal and vertical turbulent diffusion of heat and admixtures, respectively, and R is the internal heat source connected with the absorption of solar radiation.

The possibility of modeling of the transfer of substances and currents in rivers, straits, or channels with a subgrid scale in one of the horizontal directions (the width of the flow is smaller than the step of the computational grid) is attained as a result of the integration of the initial system of equations across the current (i.e., in the direction normal to the flow in the horizontal plane). The limits of integration are determined by the width of the flow (river, channel). Integration is carried out according to [120, 121, 169] under the assumption that the width of the flow B does not vary with time and depth and that the current velocity is constant in the transverse direction. A new system of equations used in the model is obtained by combining the original equations with the equations integrated across the current so that, in the absence of a channel (three-dimensional flow), the system turns into the original system of equations and, in the presence of the channel, we get the equations averaged across the flow (two-dimensional case):

$$u_t + \beta_a \{B_x^{-1}(B_x uu)_x + (uv)_y + (uw)_z\}$$

$$= -\alpha_0 P_x + fv + B_x^{-1}(2B_x A_h u_x)_x + (1-\beta_c)(A_h[v_x + u_y])_y$$

$$+ (A_v v_z)_z - \beta_c C_{ws} B_x^{-1} u|u|, \tag{3.8}$$

$$v_t + \beta_a \{(uv)_x + B_y^{-1}(B_y vu)_y + (uw)_z\}$$

$$= -\alpha_0 P_y - fu + B_y^{-1}(2B_y A_h v_y)_y + (1-\beta_c)(A_h[u_y + v_x])_x$$

$$+ (A_v v_z)_z - \beta_c C_{ws} B_y^{-1} v|v|, \tag{3.9}$$

$$B_x^{-1}(B_x u)_x + B_y^{-1}(B_y v)_y + w_z = 0, \tag{3.10}$$

$$S_t + B_x^{-1}(B_x uS - B_x D_h S_x)_x + B_y^{-1}(B_y vS - B_y D_h S_y)_y + (wS - D_v S_z)_z = 0, \tag{3.11}$$

$$T_t + B_x^{-1}(B_x uT - B_x D_h T_x)_x + B_y^{-1}(B_y vT - B_y D_h T_y)_y + (wT - D_v T_z)_z = R, \tag{3.12}$$

where B_x and B_y are the dimensionless (relative to the sizes of a cell of the computational grid) current widths in the directions x and y, respectively, β_c is a factor equal to 0 in the absence of the channel and to 1 in the presence of the channel, and C_{ws} is the coefficient of lateral friction against the walls of the channel. Equations (3.8)–(3.12) immediately turn into Eqs. (3.1), (3.2), (3.4), (3.6), and (3.7) if we set $\beta_c = 0$ and $B_x = B_y = 1$. The equations of state and hydrostatic equations remain unchanged.

For the numerical realization of the presented system of equations, it is reasonable to pass to curvilinear (in the vertical direction) coordinates (σ-system). On the one hand, this improves the computational properties of the model and, on the other hand, enables one to give a more exact description of the vertical dynamic and thermohaline structures of waters at small depths. For this purpose, we use the following transformation rectifying the bottom:

$$\sigma = \frac{z - h}{H}, \qquad H = \beta_h h + d, \tag{3.13}$$

where σ is a new coordinate varying within the range $[0, -1]$ from the surface to the bottom, H is the total local depth, d is the depth of the sea for its nondisturbed level, h is the deviation of sea level from its nondisturbed value, and β_h is a control factor (equal to 0 or 1) linearizing the influence of the total depth.

The transformation of expressions written in the coordinate system x, y, z (and denoted by $[\cdot]$) to the new coordinate system x, y, σ [in this case, we write $(\cdot)$] is realized as follows:

$$[\cdot]_z = H^{-1}(\cdot)_\sigma, \tag{3.14}$$

$$[\cdot]_x = (\cdot)_x - H^{-1}(h_x + \sigma H_x)(\cdot)_\sigma, \tag{3.15}$$

$$[\cdot]_y = (\cdot)_y - H^{-1}(h_y + \sigma H_y)(\cdot)_\sigma, \tag{3.16}$$

$$[\cdot]_t = (\cdot)_t - H^{-1}(1 + \sigma)h_t(\cdot)_\sigma. \tag{3.17}$$

To deduce an equation for the horizontal pressure gradient, it is necessary to integrate the equation of hydrostatics over the vertical. In the σ-coordinate system, this equation takes the following form:

$$P_\sigma = -\rho g H, \tag{3.18}$$

whence it follows that

$$P = gH\int_\sigma^0 \rho\, d\sigma + P_a, \tag{3.19}$$

where P_a is atmospheric pressure. In view of (3.15), we get

$$
\begin{aligned}
P_x &= P_x\Big|_{\sigma=\text{const}} - \frac{1}{H}(h_x + \sigma H_x)P_\sigma + P_{ax} \\
&= g\left(H\int_\sigma^0 \rho\, d\sigma\right)_x - \frac{1}{H}(h_x + \sigma H_x)(-\rho g H) + P_{ax} \\
&= g\left(H\int_\sigma^0 \rho\, d\sigma\right)_x + \rho g(h_x + \sigma H_x) + P_{ax}.
\end{aligned}
\tag{3.20}
$$

Note that, for $\rho = \rho_0$, we have

$$
P_x = \rho_0 g(-H_x + h_x + \sigma H_x) = \rho_0 g h_x + P_{ax}. \tag{3.21}
$$

Therefore, substituting the expression $\rho = \rho_0 + (\rho - \rho_0)$ in relation (3.20), we get

$$
\alpha_0 P_x = g h_x + G_x + \alpha_0 P_{ax}, \tag{3.22}
$$

where

$$
G_x = \alpha_0 \beta_p g \left\{ \left[H \int_\sigma^0 (\rho - \rho_0)\, d\sigma \right]_x + (h_x + \sigma H_x)(\rho - \rho_0) \right\} \tag{3.23}
$$

and β_p is a control factor (taking values 0 and 1 and used to exclude the influence of the horizontal density gradient).

In the coordinate system x, y, σ, the equations of motion take the form

$$
\begin{aligned}
&(Hu)_t + \beta_a \{B_x^{-1}(HB_x uu)_x + (Huv)_y + (u\tilde{w})_\sigma\} \\
&\quad = -gHh_x - \alpha_0 HP_{ax} - HG_x + fHv + B_x^{-1}(2HB_x A_h u_x)_x \\
&\qquad + (1-\beta_c)(A_h H[v_x + u_y])_y + H^{-1}(A_v u_\sigma)_\sigma - \beta_c C_{ws} HB_x^{-1} u|u|,
\end{aligned}
\tag{3.24}
$$

$$
\begin{aligned}
&(Hv)_t + \beta_a \{(Hvu)_x + B_y^{-1}(HB_y vv)_y + (v\tilde{w})_\sigma\} \\
&\quad = -gHh_y - \alpha_0 HP_{ay} - HG_y - fHu + B_y^{-1}(2HB_y A_h v_y)_y \\
&\qquad + (1-\beta_c)(A_h H[u_y + v_x])_x + H^{-1}(A_v v_\sigma)_\sigma - \beta_c C_{ws} HB_y^{-1} v|v|,
\end{aligned}
\tag{3.25}
$$

where

$$\tilde{w} = H\frac{d\sigma}{dt} = w - (1+\sigma)h_t - u(h_x + \sigma H_x) - v(h_y + \sigma H_y) \tag{3.26}$$

and

$$G_y = \alpha_0 g \beta_p \left\{ \left[H\int_{\sigma}^{0} (\rho - \rho_0)\, d\sigma \right]_y + g(h_y + \sigma H_y)(\rho - \rho_0) \right\}. \tag{3.27}$$

The continuity equation now takes the form

$$h_t + B_x^{-1}(HB_x u)_x + B_y^{-1}(HB_y v)_y + \tilde{w}_\sigma = 0. \tag{3.28}$$

For the equations of conservation of heat and salt, we get

$$(HS)_t + B_x^{-1}(B_x H[uS - D_h S_x])_x + B_y^{-1}(B_y H[vS - D_h S_y])_y$$
$$+ (\tilde{w}S - H^{-1}D_v S_\sigma)_\sigma = 0, \tag{3.29}$$

$$(HT)_t + B_x^{-1}(B_x H[uT - D_h T_x])_x + B_y^{-1}(B_y H[vT - D_h T_y])_y$$
$$+ (\tilde{w}T - H^{-1}D_v T_\sigma)_\sigma = HR. \tag{3.30}$$

The method used for the solution of the hydrodynamic problem is based on the decomposition of the total current velocity into the velocity averaged over depth (barotropic component) and deviations from this velocity at each depth used for computations (baroclinic component). This operation enables us to use different time steps for the barotropic and baroclinic components of the horizontal current velocity in the numerical solution of the dynamic equations because the first component is connected with the oscillations of the sea level caused by the motion of long gravitational waves and varies more rapidly than the second component.

Thus, the components of the barotropic current velocity are defined as follows:

$$U = \int_{-1}^{0} u\, d\sigma \quad \text{and} \quad V = \int_{-1}^{0} v\, d\sigma. \tag{3.31}$$

The equations of motion integrated over the vertical take the form

$$(HU)_t + \beta_a \{ B_x^{-1}(HB_x \theta_{uu} UU)_x + (H\theta_{uv} UV)_y \}$$

$$= -gHh_x - \alpha_0 HP_{ax} - HG_x^* + fHV + B_x^{-1}(2A_h HB_x U_x)_x$$

$$+ (1-\beta_c)\big(A_h H[V_x + U_y]\big)_y + \tau_{sx} - \tau_{bx} - \beta_c C_{ws} B_x^{-1} H\theta_{su} U|U|, \quad (3.32)$$

$$(HV)_t + \beta_a\{(H\theta_{uv}UV)_x + B_y^{-1}(HB_y\theta_{vv}VV)_y\}$$

$$= -gHh_y - \alpha_0 HP_{ay} - HG_y^* - fHU + B_y^{-1}(2A_h HB_y V_y)_y$$

$$+ (1-\beta_c)\big(A_h H[V_x + U_y]\big)_x + \tau_{sy} - \tau_{by} - \beta_c C_{ws} B_y^{-1} H\theta_{sv} V|V|, \quad (3.33)$$

where

$$G_x^* = \int_{-1}^{0} G_x\, d\sigma, \qquad G_y^* = \int_{-1}^{0} G_y\, d\sigma,$$

$$\theta_{uu} = \int_{-1}^{0} \frac{uu}{UU}\, d\sigma, \qquad \theta_{uv} = \int_{-1}^{0} \frac{uv}{UV}\, d\sigma, \qquad \theta_{vv} = \int_{-1}^{0} \frac{vv}{VV}\, d\sigma,$$

$$\theta_{su} = \int_{-1}^{0} \left(\frac{u}{U}\right)\left|\frac{u}{U}\right| d\sigma, \qquad \theta_{sv} = \int_{-1}^{0} \left(\frac{v}{V}\right)\left|\frac{v}{V}\right| d\sigma.$$

The continuity equation for the barotropic components now takes the form

$$h_t + B_x^{-1}(B_x HU)_x + B_y^{-1}(B_y HV)_y = 0. \quad (3.34)$$

The baroclinic components of the vector of current velocity are determined as deviations from the velocity averaged over the depth:

$$u' = u - U \quad \text{and} \quad v' = v - V. \quad (3.35)$$

The equations for these components are obtained by subtracting the equations for the barotropic component of the velocity from the equations for the total velocity:

$$(Hu')_x + \beta_a\{B_x^{-1}(B_x H[uu - \theta_{uu}UU])_x + \big(H[uv - \theta_{uv}UV]\big)_y + (\tilde{w}u')_\sigma\}$$

$$= HG_x^* - HG_x + fHv' + B_x^{-1}(2A_h HB_x u'_x)_x + (1-\beta_c)\big(A_h H[v'_x + u'_y]\big)_y$$

$$+ H^{-1}(A_v u'_\sigma)_\sigma - \tau_{sx} + \tau_{bx} - \beta_c C_{ws} H B_x^{-1}(u|u| - \theta_{su}U|U|), \quad (3.36)$$

$$(Hv')_t + \beta_a \{B_y^{-1}(B_y H[vv - \theta_{vv} VV])_x + (H[uv - \theta_{uv} UV])_y + (\tilde{w}v')_\sigma\}$$

$$= HG_y^* - HG_y - fHu' + B_y^{-1}(2A_h HB_y v'_y)_y + (1 - \beta_c)(A_h H[v'_x + u'_y])_x$$

$$+ H^{-1}(A_v v'_\sigma)_\sigma - \tau_{sy} + \tau_{by} - \beta_c C_{ws} HB_y^{-1}(v|v| - \theta_{sv} V|V|). \qquad (3.37)$$

The continuity equation for the baroclinic component is represented in the form

$$B_x^{-1}(B_x Hu')_x + B_y^{-1}(B_y Hv')_y + H^{-1}(\tilde{w})_\sigma = 0. \qquad (3.38)$$

3.1.1. Parametrizations of the Processes Used in the Model

The Coriolis acceleration f is given by the formula

$$f = f_c + (f_x)\big|_{x=x_c}(x - x_c) + (f_y)\big|_{y=y_c}(y - y_c), \qquad (3.39)$$

where f_c is the initial value of the parameter at a point with known latitude and longitude corresponding to a node of the computational grid.

The equation of state is represented in the form

$$\rho = \rho_0[1 + F_\rho(S, T)], \qquad (3.40)$$

$$F_\rho = C_{S0} + C_{S1}S + C_{ST}ST + C_{T1}T + C_{T2}T^2, \qquad (3.41)$$

where S is the level of salinity (ppt), T is the temperature of water (°C), and C_{S0}, C_{S1}, C_{ST}, C_{T1}, and C_{T2} are, respectively, the coefficients equal to 0.00007, $0.000802\ \text{ppt}^{-1}$, $-0.000002\ (\text{ppt}\cdot\text{deg})^{-1}$, $-0.0000035\,°\text{C}^{-1}$, and $-0.00000469\,°\text{C}^{-2}$.

It is assumed that the vertical density distribution must be at least neutrally stable, i.e.,

$$\rho_\sigma \le 0. \qquad (3.42)$$

By using (3.40), we can find the difference of densities for two layers located along the vertical as follows:

$$\delta F_\rho = (F_\rho)_S\,\delta S + (F_\rho)_T\,\delta T, \qquad (3.43)$$

where δS and δT are, respectively, the differences between the values of temperature and salinity for these layers. Relation (3.43) gives a more exact result than just the difference between the values of density.

The wind stresses on the upper (air–water) boundary are given by the formulas

$$\tau_{sx} = (C_{aw1} + C_{aw2} W_{10}) W_{10} W_x, \tag{3.44}$$

$$\tau_{sy} = (C_{aw1} + C_{aw2} W_{10}) W_{10} W_y, \tag{3.45}$$

where W_x and W_y are the components of the wind velocity at a height of 10 m over the sea level along the x- and y-axes, respectively, W_{10} is the modulus of wind velocity at a height of 10 m, and C_{aw1} and C_{aw2} are the friction coefficients set equal to 0.0008 and 0.000065 sec/m, respectively.

The bottom friction stresses acting on the lower (water–bottom) boundary have the form

$$\tau_{bx} = \Phi u_b \quad \text{and} \quad \tau_{by} = \Phi v_b,$$

where

$$\Phi = [C_{wb1} + C_{wb2} (u_b^2 + v_b^2)^{1/2}], \tag{3.46}$$

u_b and v_b are the components of the bottom current velocity, and C_{wb1} and C_{wb2} are the friction coefficients whose typical values are equal to 0.001 and 0.0026 m/sec, respectively.

The vertical turbulent viscosity is described on the basis of the semiempirical theory of turbulence by using the length of the mixing path. The instantaneous viscosity is determined as a function of the length of the mixing path, local vertical shifts of the velocity, and stability of the water column:

$$A_v = A_{v0} + A_z [C_{R0} (1 + C_{R1} R_i)^{-C_{R2}}], \tag{3.47}$$

$$D_v = D_{v0} + A_z [C_{R3} (1 + C_{R4} R_i)^{-C_{R5}}], \tag{3.48}$$

where

$$A_z = \left[\kappa z \left(1 - \frac{z}{H}\right)\right]^2 (u_z'^2 + v_z'^2)^{1/2}, \tag{3.49}$$

$\kappa = 0.4$ is the von Kárman constant, A_{v0} is the threshold viscosity, D_{v0} is the threshold diffusion, C_{R0}, C_{R1}, C_{R2}, C_{R3}, C_{R4}, and C_{R5} are constants equal to 1.0, 10.0, 0.5, 1.0, 3.33, and 1.5, respectively [148], and the Richardson number

$$R_i = -\frac{\rho_z' g}{\rho_0 (u_z'^2 + v_z'^2)}. \tag{3.50}$$

The coefficients of horizontal turbulent exchange are found according to the values of the local horizontal shift of the barotropic component of current velocity and the space step ΔL of the horizontal finite-difference grid [158]:

$$A_h = A_{h0} + C_{AH}\Delta L^2[2(U_x^2 + V_y^2) + (U_y + V_x)^2]^{1/2}, \tag{3.51}$$

$$D_h = A_h, \tag{3.52}$$

where $C_{AH} = 0.1$ and $A_{h0} = 1.0\,\mathrm{m}^2/\mathrm{sec}$ is the background quantity.

3.1.2. Possible Simplifications of the Complete Equations of Hydrodynamic Model

The deduced complete equations of the proposed model can be somewhat simplified by specifying several sets of parameters, including the control factors.

Linearization. The terms introduced to describe nonlinear advective accelerations in Eqs. (3.32), (3.33), (3.36), and (3.37) can be excluded by setting $\beta_a = 0$. The tidal effects and surges are removed if we set $\beta_h = 0$ in Eq. (3.13) for the total depth. For the complete linearization, it is also necessary to exclude nonlinearities from Eqs. (3.46), (3.47), and (3.51) for the bottom stresses and horizontal and vertical viscosity by setting

$$C_{wb2} = 0, \quad C_{AH} = 0, \quad \text{and} \quad C_{R0} = 0.$$

Uniformity of the Density Field. In the equation of state (3.40), to exclude the influence of spatial inhomogeneities of density on the dynamics of waters, we set

$$C_{S1} = C_{ST} = C_{T1} = C_{T2} = 0.$$

Moreover, in relations (3.23) and (3.27), we set $\beta_p = 0$. In this case, the Richardson number [Eq. (3.50)] is automatically equal to zero.

Stationarity of the Density Field. This means that

$$S_t = 0 \quad \text{and} \quad T_t = 0.$$

The validity of this condition is guaranteed by excluding Eqs. (3.29) and (3.30) from the model.

Elimination of Density. The mathematical structure of the model makes it possible to perform the numerical analysis of the dynamics of waters for the distribution of temperature and salinity stationary in time but variable over the space. In this case, the thermohaline component of the current velocity is found in the diagnostic mode (by taking into account the horizontal and vertical density gradients) and all other components are computed in the prognostic mode.

The contribution of temperature and salinity to the formation of space density gradients affecting the computed field of currents can be separated or completely removed in the following way: To remove the contribution of salinity, it is necessary to set $C_{S1} = 0$ in Eq. (3.41). The contribution of temperature is eliminated if we set $C_{T1} = C_{T2} = 0$ in the same equation.

The contribution of the thermohaline factor to the formation of the fields of currents is completely eliminated by setting $C_{S1} = C_{ST} = C_{T1} = C_{T2} = 0$ and, in addition, $\beta_p = C_{R1} = C_{R4} = 0$.

3.1.3. Boundary and Initial Conditions

On the open sea boundary, we either specify the disturbances of the sea level induced, e.g., by the tides, surges, etc., i.e.,

$$h = h_a(x, y, t) \tag{3.53a}$$

or impose the radiation condition of free propagation of long gravitational waves through the boundary

$$h = h_a + \vec{V}_n \sqrt{\frac{H}{g}}, \tag{3.53b}$$

where h_a is the disturbance of level on the liquid boundary of the computational domain specified according to the data of observations or calculations and $\vec{V}_n$ is the projection of the current vector computed at the boundary points of the domain onto the outer normal $\vec{n}$ to the open lateral boundary.

For temperature and salinity, the conditions are formulated as follows: if the current comes into the analyzed region, then, on the open-sea boundary, we specify the background values of temperature and salinity (T^*, S^*) typical of the open sea; otherwise, the values of modeled variables are extrapolated from the analyzed region by using the simplified advection equation:

$$\begin{aligned} &T_a = T^* \quad \text{and} \quad S_a = S^* \quad \text{for} \quad \vec{v}_n \le 0, \\ &T_{0`t} = -\vec{v}_n T_n \quad \text{and} \quad S_{0`t} = -\vec{v}_n S_n \quad \text{for} \quad \vec{v}_n > 0, \end{aligned} \tag{3.54}$$

where T_0 and S_0 are the values of modeled variables on the open-sea boundary. Furthermore, if the current is directed into the computational region for less than 6 h, then we use the following interpolation scheme:

$$(S_0, T_0) = F_i(S^*, T^*) + (1 - F_i)(S_0, T_0), \tag{3.55}$$

where F_i is the ratio of the time step for the baroclinic component of the velocity (in hours) to the difference between 6 h and the time period of penetration of the current into the analyzed region, $0 \le F_i \le 1$.

At the points of inflow of rivers, we impose either the open-channel- or waterfall-type boundary conditions. In the first case, we specify the flow rates Q_r and the vertical profiles of baroclinic velocity, temperature, and salinity, i.e.,

$$U = \frac{Q_r}{B_x \Delta L H}, \qquad V = \frac{Q_r}{B_y \Delta L H}, \tag{3.56}$$

$$u' = u_{\text{top}} \cos\left(\frac{\pi z}{H}\right), \qquad v' = v_{\text{top}} \cos\left(\frac{\pi z}{H}\right), \tag{3.57}$$

$$\begin{aligned} S &= S_{\text{top}} + (S_{\text{top}} - S_{\text{bot}})\left[1 - \cos\left(\frac{\pi z}{H}\right)\right], \\ T &= T_{\text{top}} + (T_{\text{top}} - T_{\text{bot}})\left[1 - \cos\left(\frac{\pi z}{H}\right)\right], \end{aligned} \tag{3.58}$$

where the subscripts “top” and “bot” correspond to the surface and bottom layers of water, respectively.

The waterfall-type boundary conditions have the following form:

$$h_t = \frac{Q_r}{B_x B_y \Delta L^2}, \tag{3.59}$$

$$(HS)_t = 0, \quad \text{and} \quad (HT)_t = \frac{T_{\text{top}} Q_r}{B_x B_y \Delta L^2}. \tag{3.60}$$

On the sea surface, we set

$$\tau_{sx} = A_v u'_z, \quad \tau_{sy} = A_v v'_z, \quad D_v T_z = \frac{Q_T}{\rho C_w}, \quad \text{and} \quad D_v S_z = 0 \tag{3.61}$$

and, at the bottom,

$$\tau_{bx} = A_v u'_z, \quad \tau_{by} = A_v v'_z, \quad D_v S_z = 0,$$

$$\text{and} \quad D_v T_z = [C_{\text{bed}1} + C_{\text{bed}2}(u_b^2 + v_b^2)^{1/2}](T_{\text{bed}} - T), \tag{3.62}$$

where τ_{sx} and τ_{sy} are the components of the vector of tangential wind stresses, τ_{bx} and τ_{by} are the components of the vector of tangential bottom friction stresses, Q_T is the heat flux computed according to the meteorological data, C_w is the specific heat capacity of water, $C_{\text{bed}1}$ and $C_{\text{bed}2}$ are the exchange coefficients set equal to 0.000001 m/sec and 0.003, respectively, and T_{bed} is the temperature of the bottom.

As the initial conditions, we take the state of rest, i.e.,

$$U = V = u' = v' = w = 0, \quad A_h = A_{h0}, \quad A_v = A_{v0}, \quad D_v = D_{v0}. \tag{3.63}$$

The initial values of temperature, salinity, and the sea level at the internal points of the analyzed region are found as a result of interpolation of the boundary values with weights inversely proportional to the distance from the boundary. The temperature of the bottom sediments T_{bed} is also specified.

To improve the computational stability, we assume that the Coriolis acceleration, wind stresses, and horizontal gradients of the atmospheric pressure and density on the open sea boundaries are equal to zero. In this case, we use a special multiplicative boundary function equal to zero in the computational cells located on the boundary, to 0.5 in the cells adjacent to the boundary cells, and to 1 in all other cells.

The nonlinear advective terms of the equations of motion are also set equal to zero on the open sea boundary.

3.1.4. Block of Heat Exchange with the Atmosphere

The total specific heat flux Q_T incident on the air–water interface can be represented as the sum of two components:

$$Q_T = Q_1 + Q_2, \tag{3.64}$$

where Q_1 is the short-wave component of solar radiation penetrating in the water column through the surface and Q_2 is the long-wave radiation absorbed by the surface.

The specific flux of short-wave radiation Q_1 is used to find the internal heat source R (°C/sec) in the layer:

$$R = \frac{Q_1}{\rho C_w} \frac{1}{z_b - z_a} \left[\exp\left\{ \frac{2.3 z_a}{D_{10}} \right\} - \exp\left\{ \frac{2.3 z_b}{D_{10}} \right\} \right], \tag{3.65}$$

where z_a and z_b are the z-coordinates of upper and lower boundaries of the layer, respectively, and D_{10} is the depth of penetration of 10% of the flux incident on the sea surface. It is also assumed that the initial flux exponentially decreases with depth and, hence, the attenuation factor is specified as follows: $2.3/D_{10}$.

The short-wave component of the specific solar heat flux is given by the formula

$$Q_1 = Q_{ss}(1 - A_{1b})F_{cc}(C_c), \tag{3.66}$$

where Q_{ss} is the flux coming to the sea surface under the conditions of cloudiness, A_{1b} is the albedo of the sea surface, F_{cc} is a function of cloudiness, and C_c is a part of the sky covered with clouds.

According to [84],

$$Q_{ss} = \frac{C_{\text{sol}}\cos^2(\zeta)}{0.10 + 1.085\cos(\zeta) + 10^{-5}\{\cos(\zeta) + 2.7\}e_v}, \tag{3.67}$$

where C_{sol} is the solar constant (1353 W/m^2), e_v is the pressure of water vapor, and ζ is the zenith angle of the Sun given by the formula

$$\cos(\zeta) = \sin(\lambda_a)\sin(\varphi) + \cos(\lambda_a)\cos(\varphi)\cos(\nu). \tag{3.68}$$

Here, λ_a is the geographic latitude,

$$\varphi = 23.44°\cos\left(\frac{2\pi[172 - N\text{day}]}{365}\right)$$

is the declination, Nday is the number of a day in the year,

$$\nu = \frac{2\pi(12 - Shr)}{24}$$

is the hour angle, and Shr is the solar hour, i.e., the hour of a day.

For the pressure of water vapor e_v, we can write

$$e_v = R_h e_s(T), \tag{3.69}$$

where R_h is the relative humidity and e_s is the saturating pressure of water vapor (mbar) given by the formula [84]:

$$e_s(T) = 611\cdot 10^{(7.5[T - 273.16]/[T - 35.86])}. \tag{3.70}$$

In relation (3.69), the pressure of water vapor e_v is found for the air temperature T_{a0} (°K) on the air–water interface.

The function of cloudiness is determined as follows:

$$F_{cc}(C_c) = 1 - C_c. \tag{3.71}$$

The heat flux on the air–water interface can be represented in the form of a sum of several components:

$$Q_2 = Q_L + Q_B + Q_e + Q_s, \tag{3.72}$$

where Q_L is the long-wave radiation of the atmosphere, Q_B is the backward radiation of the black body by the sea surface, Q_e are the heat losses for evaporation, and Q_s is the heat flux of contact heat exchange between the sea and the atmosphere. These quantities are given by the following formulas:

$$Q_L = C_{sb} T_a^4 \left(1 - 0.26 \exp[-0.000777(273 - T_a)^2]\right), \tag{3.73}$$

where C_{sb} is the Stefan–Boltzmann constant $(5.67 \cdot 10^{-8}\ \mathrm{W/(m^2 \cdot {}^\circ K^4)})$ and T_a is the observed air temperature (°K);

$$Q_B = -0.97 C_{sb} \left(T|_{\sigma=0}\right)^4, \tag{3.74}$$

where 0.97 is the emissivity of the surface;

$$Q_e = -0.00175 \rho_a L_y W_{10} (\gamma_{10} - \gamma_0), \tag{3.75}$$

where ρ_a is the density of air, W_{10} is the wind velocity at a height of 10 m, γ_{10} and γ_0 are the values of relative humidity at a height of 10 m and on the sea surface, respectively, L_y is the latent heat of evaporation $(2.5 \cdot 10^6$ J/kg), the relative humidity is expressed via the pressure of water vapor by the formula

$$\gamma = \frac{0.622 e_v}{P_a - (1 - 0.622) e_v}, \tag{3.76}$$

where 0.622 is the ratio of the molecular weights of water vapor and dry air, and P_a is the atmospheric pressure (mbar);

$$Q_s = 0.00175 \rho_a c_p W_{10} (T_{a10} - T_{a0}), \tag{3.77}$$

where c_p is the specific heat capacity of dry air (1004 J/kgK) and T_{a10} and T_{a0} are, respectively, the air temperatures at a height of 10m and on the sea surface. It is assumed that the air and water temperatures are equal on the sea surface and, hence, $T_{a0} = T|_{\sigma=0}$ and $T_{a10} = T_a$.

3.2. Block of Transfer of Admixtures

The chemical-and-biological part of the model is combined with the hydrodynamic block into a single model of the quality of waters on the basis of the equation of nonconservative transfer of admixtures. The structure of this equation is similar to structure of the equations of conservation of heat and salt (3.11)–(3.12) and (3.29)–(3.30) of the hydrodynamic model but differs from these equations by the presence of the gravitational velocity of sedimentation of admixtures and the form of the right-hand side introduced to describe the nonconservative behavior of admixtures. In the σ-coordinate system, the generalized equation of transfer of admixtures takes the following form:

$$(HC_i)_t + B_x^{-1}(B_x H[uC_i - D_h(C_i)_x])_x + B_y^{-1}(B_y H[vC_i - D_h(C_i)_y])_y$$

$$+ ((\tilde{w} + w_{gi})C_i - H^{-1}D_v(C_i)_\sigma)_\sigma$$

$$= HF_i(\vec{C}, x, y, z, t)_i + HQ_i(x, y, z, t), \quad (3.78)$$

where $\vec{C}$ is the vector function of the variables of state of the ecosystem $(i = 1, 2, 3, \dots, N)$ whose elements are the concentrations (biomass) C_i of modeled components of the ecosystem or pollutants, w_{gi} is the velocity of gravitational sedimentation of admixtures, F_i is the function of nonconservatism of the ith admixture (substance) used to describe the chemical and biological processes of its transformation

$$\frac{\partial C_i}{\partial t} = F_i,$$

and Q_i is the inflow of the substances from the external sources (including the sources of the anthropogenic origin).

Depending on the type of analyzed substances, the functions of nonconservatism F_i are determined in the blocks of self-cleaning or eutrophication. For each time step, we solve the system of equations of transfer of nonconservative substances. The number of equations similar to (3.78) in this system corresponds to the number of modeled variables of state of the ecosystem or the kinds of pollutants.

The boundary conditions imposed on the process of transfer of admixtures have the form:

$$w_{gi}C_i - D_v(C_i)_z = Q_{ci}^{\text{top}}, \quad (3.79)$$

on the sea surface,

$$w_{gi}C_i - D_v(C_i)_z = Q_{ci}^{\text{bot}}, \quad (3.80)$$

at the bottom

$$C_{oi} = C_i^* \quad \text{for} \quad \vec{v}\vec{n} \le 0 \quad \text{and} \quad \frac{\partial C_{oi}}{\partial t} = -\vec{v}\vec{n}\frac{\partial C_i}{\partial \vec{n}} \quad \text{for} \quad \vec{v}\vec{n} > 0, \quad (3.81)$$

on the lateral “liquid” boundary,

$$C_i^R = C_i^{\text{top}} + (C_i^{\text{top}} - C_i^{\text{bot}})\left(1 - \cos\frac{\pi z}{H}\right), \tag{3.82}$$

at the points of inflow of rivers on the solid boundary, and

$$(HC_i)_t = \frac{C_i^a Q_{ai}}{B_x B_y \Delta L^2}. \tag{3.83}$$

at the points of location of the anthropogenic sources of pollution. Here, Q_{ci}^{top} is the flux of admixtures through the water surface, Q_{ci}^{bot} is the flux of admixtures through the "water–bottom sediments" boundary, C_{oi} is the concentration of the ith admixture on the open-sea boundary, C_i^a and Q_{ai} are, respectively, the concentration of the same admixture in the waste waters of an anthropogenic source of pollution and its flow rate, and C_i^* is the background concentration of admixture typical of the open sea.

For the specific types of modeled substances, the fluxes Q_{ci}^{top} and Q_{ci}^{bot} are specified or computed in the chemical-and-biological block of the model.

3.3. Specific Features of Numerical Realization of the Model Equations

The finite-difference approximation of equations (3.32)–(3.34) for the barotropic mode of motion is realized on the basis of the two-step three-layer (in time) version of the Abbot alternating-direction method [157]. We use the values of computed quantities (h, U, and V) corresponding to three time points within the step Δt for the barotropic mode of motion: initial (t_0), precomputed $(t_0 + \Delta t)$, and intermediate $(t_0 + \Delta t/2)$. In the first step, as a result of the simultaneous solution of the equations of continuity and motion along the x-axis, we find the values of U for the precomputed time point and h for the intermediate point. In the second step, we solve the equations of continuity and motion along the y-axis and determine the values of V and h for the precomputed time points $(t_0 + \Delta t)$. The indicated numerical method of solution belongs to the class of implicit methods.

The location of variables inside an elementary cell of the computational grid is shown in Fig. 3.1 and the location of an elementary cell inside a segment of the computational region is presented in Fig. 3.2.

Equations (3.36)–(3.38) for the baroclinic mode of motion are solved implicitly by the sweep method (along the vertical coordinate). For this purpose, the terms containing time or the derivative of the velocity with respect to the vertical coordinate and the term taking into account the lateral friction are grouped on the left-hand side of the equation. Thus, Eq. (3.36) now takes the form

$$(Hu')_t + \beta_a\{(\tilde{w}u')_q\} - H^{-1}(A_v u'_q)_q + \beta_c C_{ws} H B_x^{-1} u' |u' + U| = R, \tag{3.84}$$

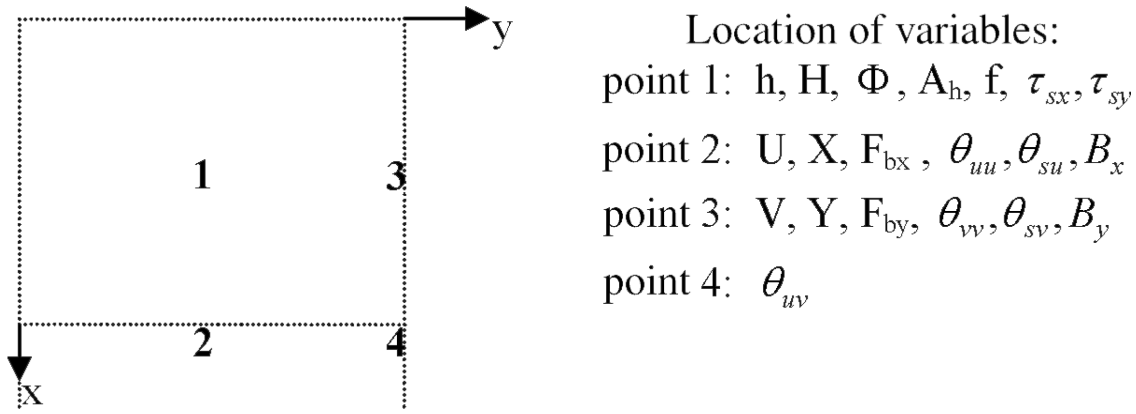


Fig. 3.1. Location of variables inside an elementary cell of the computational grid in the horizontal plane.

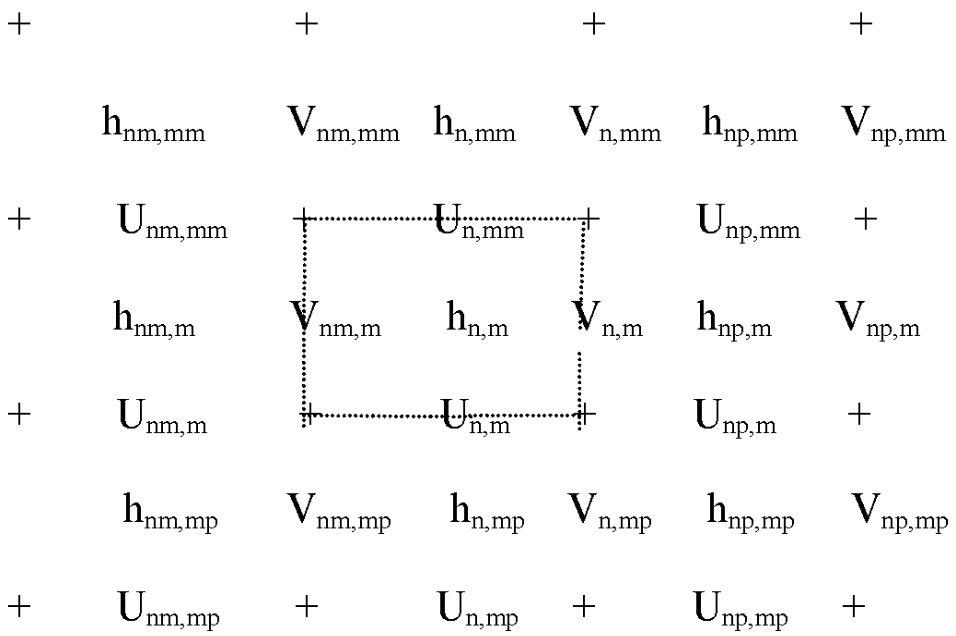


Fig. 3.2. Location of the variables U, V, and h inside a fragment of the analyzed region. The dotted lines mark the cell (n, m). Here, we use the following notation: $mm = m - 1$, $mp = n + 1$, $nm = n - 1$, and $np = n + 1$.

where R is its remaining part of the equation.

The general approach to the solution of the problem can be described as follows: first, we determine u' and v' at all vertical levels of an elementary computational cell and, then pass to the next cell and repeat the procedure.

In Fig. 3.3, we show the location of the nodes used to compute u', v', $\tilde{w}$, and A_v on a vertical fragment of the computational grid.

Since the methods used for the numerical solution of the hydrodynamic equations of the model are implicit, these solutions are computationally stable for the major part of practical cases.

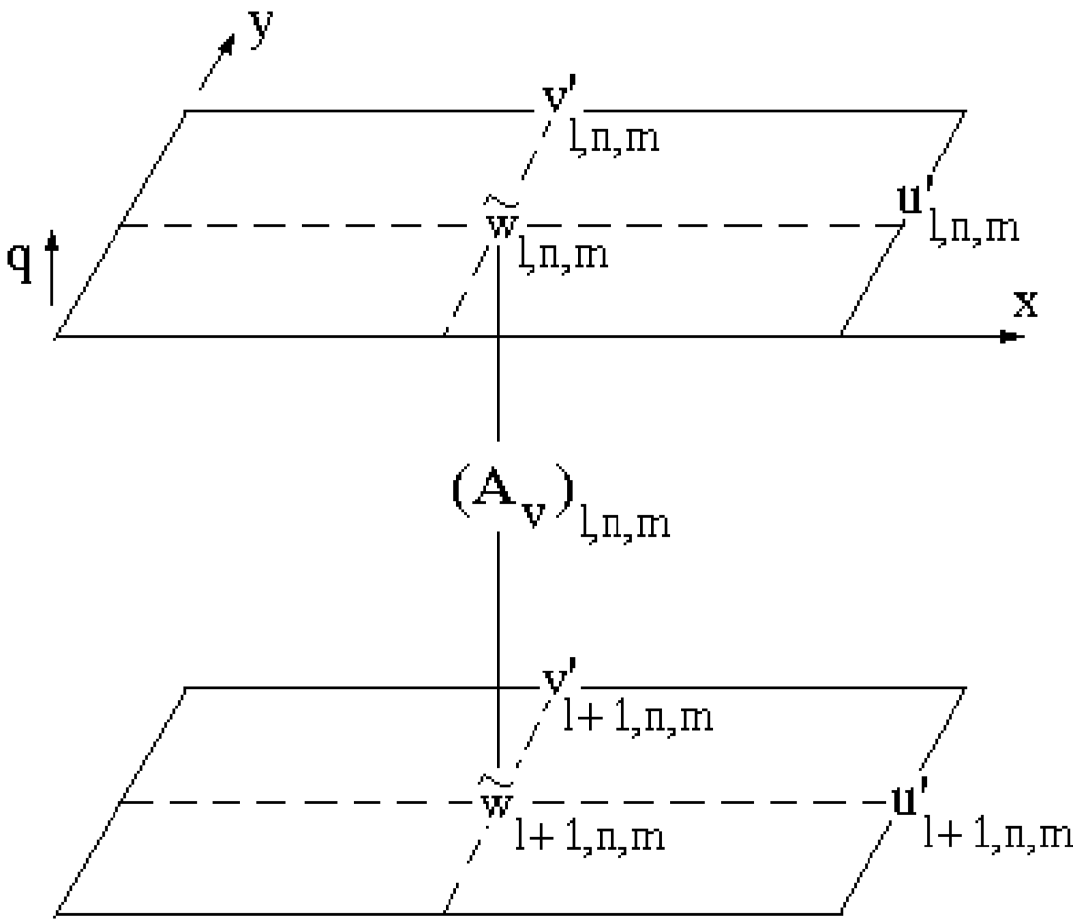


Fig. 3.3. Location of the nodes used to compute u', v', $\tilde{w}$, and A_v in the three-dimensional computational grid.

The finite-difference approximation of the equations of heat and salt transfer in the original version of the MECCA model is realized by using the traditional algorithms of the numerical solution (by using simple approximations of the derivatives) [138]. These algorithms are conservative but do not possess the property of transportivity (monotonicity). In the presence of significant space gradients of modeled elements (in the estuary regions) on the scales comparable with the step of the computational grid, this may lead to the appearance of negative values of concentrations in the process of numerical calculations, which is undesirable in the solution of ecological problems. Therefore, the original numerical schemes of the solution of transfer equations of the form (3.29), (3.30), and (3.78) are modified into transportive schemes, i.e., into the FCT (Flux Corrected Transport) scheme [110, 124] for the horizontal transfer and the TVD (Total Variation Diminishing) scheme [110] for the vertical transfer.

The details of numerical realization of the hydrodynamic equations of the model can be found in [139] and the modifications of the transfer equations are discussed in [153].

The software realization of the model in the FORTRAN-90 language enables us both to compute the resulting currents and separate their wind, thermohaline, and sink components. In the course of numerical analysis with given time steps, the model assimilates new data on the velocity and direction of the wind, air temperature, river discharge, temperature and salinity of river waters, thermohaline stratification, disturbances of the sea level at some points of the sea boundary, concentrations of admixtures in river waters and waste waters from the anthropogenic sources of pollution, and background concentrations on the open sea boundary. Further, we perform the linear interpolation of the introduced discrete values: In time, for the meteorological parameters and the parameters of rivers or in space and time, for the disturbances of the sea level, concentrations of admixtures, and the vertical distributions of temperature and salinity of water on the open boundaries.

The model enables one to compute the space-and-time variations of modeled characteristics on scales from several hours to several years and from several hundred meters to tens of kilometers. It can be used both in the shelf and estuary zones of the sea with depths from several meters to several hundred meters (with regard for the thermohaline stratification) and in the shallow-water parts of the sea, firths, bays, and river mouths with depths of several decimeters and greater (without taking into account the thermohaline stratification and the corresponding component of currents).

3.4. Results of Adaptation of the Hydrodynamical Model to the Conditions Formed in the Northwest Part of the Black Sea

The northwest part of the Black Sea has the own specific features distinguishing it from the other parts of the sea. Thus, we can mention, first, the fact that this is a shallow-water region and, hence, the wind component is predominant in the formation of the circulation of waters and, second, the presence of estuary regions of four large rivers (Danube, Dnieper, Yuzhnyi Bug, and Dniester). The freshwater discharge of these rivers exerts a significant influence on the formation of the thermohaline structure and specifies the density component of the currents. The northwest part of the Black Sea is characterized by the strong irregularity of the coastal line with numerous shallow-water bays (Zhebriyanskii, Odesskii, Egorlytskii, Tendrovskii, and Dzharylgachskii) and firths (Sukhoi, Dnestrovskii, Dneprovsko-Bugskii, and Grigor'evskii) connected with the open sea via narrow straits. In many cases, bays and firths can, in fact, be regarded as parts of the estuary regions of rivers (Zhebriyanskii Bay, Dnestrovskii Firth, and Dneprovsko-Bugskii Firth).

In spring and summer, the hydrochemical conditions formed in the water area of the northwest part of the Black Sea are strongly affected by the development of sharpened seasonal pycnocline caused by the process of heating of surface waters and their freshening by river waters against the general background of seasonal weakening of the intensity of winds.

According to [95], in the formation of the jump of density in the northwest part of the Black Sea in spring and summer, the thermal causes play a more significant role than the freshening effect of rivers everywhere except the estuary regions. The pycnocline is formed as a result of spring and summer heating of the surface layer and wind-wave mixing, whereas the process of freshening only strengthens the general stratification and forms a single jump of density.

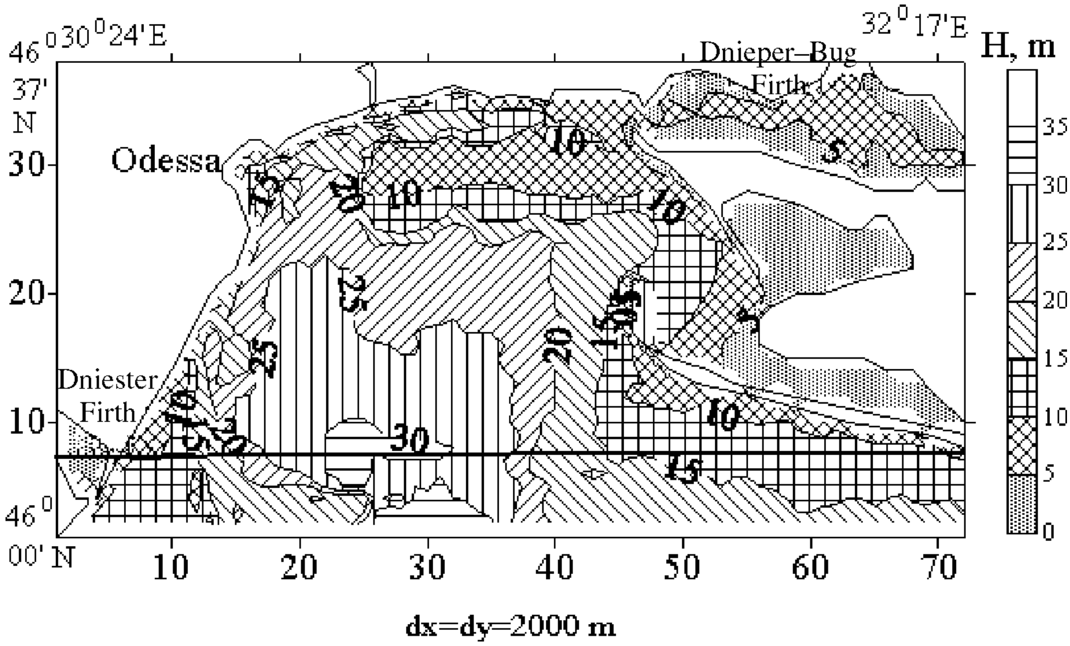


Fig. 3.4. Dnieper–Bug near estuary and Odessa regions in the northwest part of the Black Sea (the depths are measured in meters). The solid line marks the lower boundary of the computational region used in the model of the quality of waters (the discharge of Dniester is not taken into account).

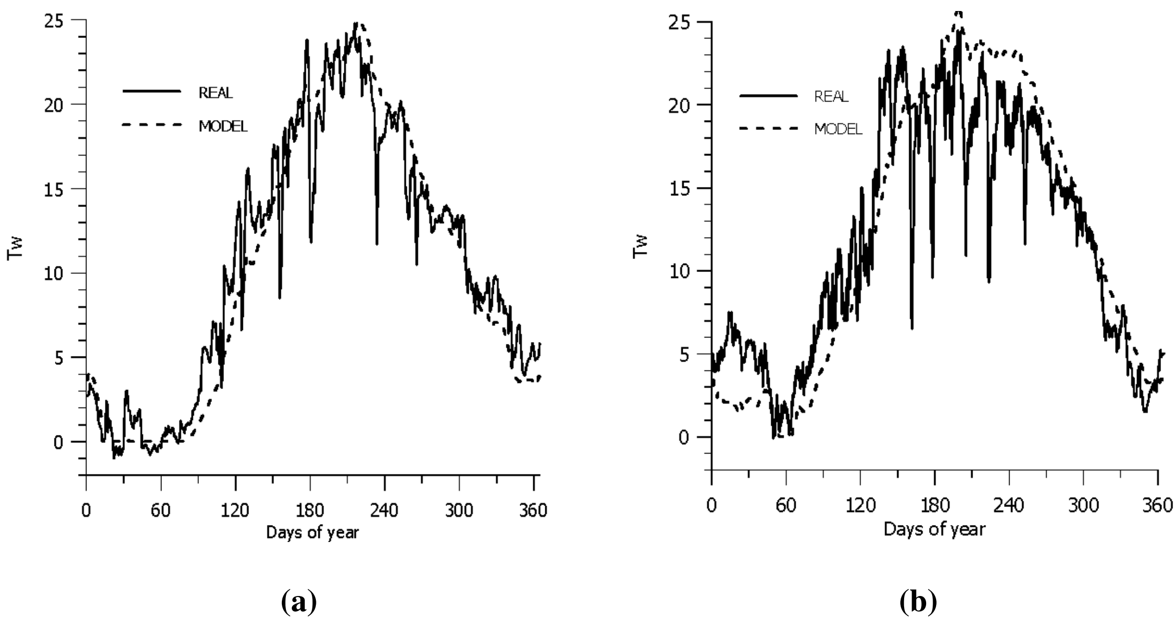


Fig. 3.5. Measured (solid line) and computed according to the one-dimensional version of the model (dotted line) annual courses of temperature of the surface layer of water (°C) in 1981 (a) and 1983 (b).

The indicated morphological and hydrological specific features of the northwest part of the Black Sea enable us to use this example for the convincing demonstration of the adequacy of description of natural processes by the hydrodynamical model, its informativity and computational possibilities. In what follows, we present the results of adaptation and verification of the proposed hydrothermodynamic model to the conditions of the Dnieper–Bug estuary region in the northwest part of the Black Sea and the Odessa region regarded as its constituent part.

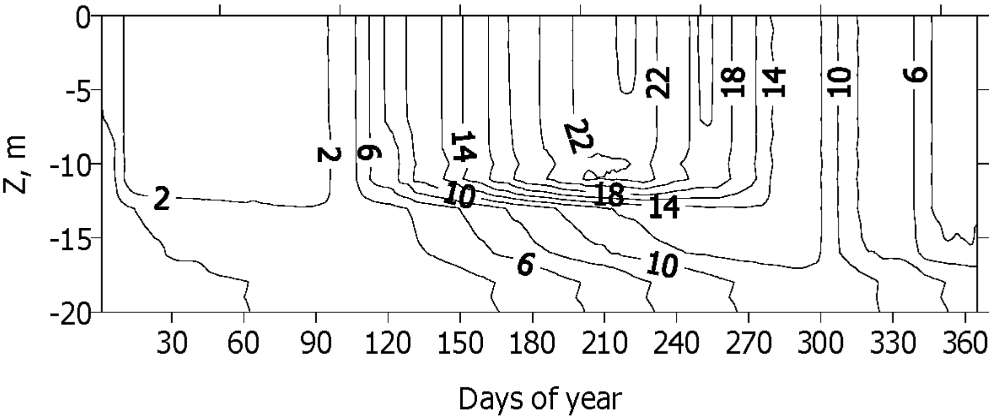
In the first series of numerical experiments, the computational region was approximated by a space grid with 68×32 nodes and steps of 2000 m (in Fig. 3.4, the south boundary of this region is marked by the solid line). The time steps were equal to 6 and 72 sec for the barotropic and baroclinic components of the current velocity, respectively. In numerical calculations, we used ten levels of depth in the σ-system of coordinates.

Initially, the model was tested in the one-dimensional version (in the vertical direction) in which the terms of equations used to describe the horizontal turbulent exchange and advective transfer were neglected and all functions were regarded as independent of the horizontal coordinates. In this statement, we take into account solely the baroclinic wind component of the current velocity used for the evaluation of the coefficients of vertical turbulent exchange and diffusion. Thus, we actually solve the problem of formation of the vertical thermal (thermohaline) structure of waters as a result of both the vertical turbulent exchange of momentum and the diffusion of heat (and salts).

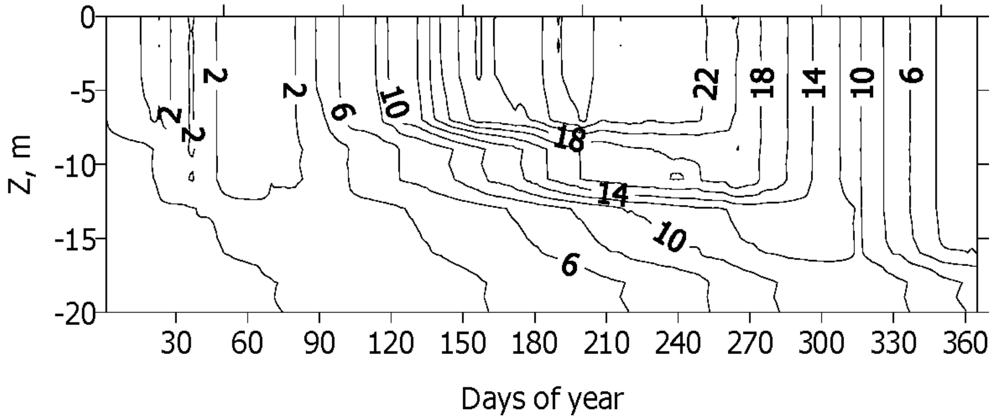
The purpose of numerical calculations is to study the possibility of reconstruction by the model of the annual variability of the vertical thermohaline structure of waters under the action of the wind and heat exchange with the atmosphere. As the initial data, we use the results of regular 6-h observations over the air temperature and the velocity and direction of winds regularly carried out by the "Odessa-port" hydrometeorological station. In our calculations, the annual course of the monthly average values of salinity in the surface and bottom layers of the water column is specified according to the data presented in [14, 21]. The vertical distribution of salinity is determined in the course of numerical calculations (Figs. 3.4–3.6).

The accumulated numerical results show that the model correctly describes the annual course of temperature in the surface layer of waters and the processes of formation and destruction of the seasonal thermocline. We reveal certain distinctions between the numerical results and the data of observations. Indeed, in the summer months, the computed temperature of the surface layer exceeds, in numerous cases, the observed values of temperature by several degrees. Moreover, in the spring and summer months, the bottom layer is heated slower than it follows from the data of observations. However, these disagreements are, to a significant extent, caused by the elimination of the contribution of horizontal advection of waters to the heat exchange between the surface and bottom water masses (due to the surge phenomena).

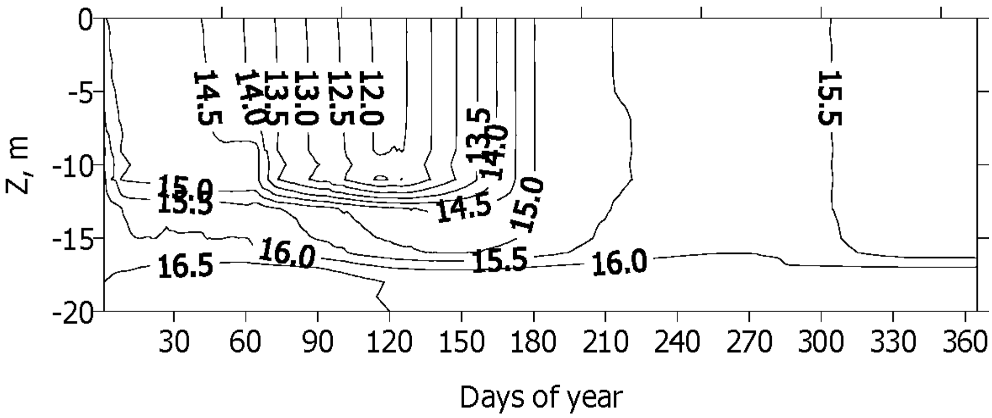
The other series of numerical experiments carried out with the three-dimensional version of the model is aimed at the analysis of variations of the three-dimensional thermohaline structure of waters and the field of currents under constant wind conditions in the period of spring flood when the contribution of the thermohaline factor to the dynamics of waters is maximum. In our case, the numerical analysis is aimed at the reconstruction of the process of propagation of the tongue of freshened waters from the Dnieper –Bug Firth into the Odessa region of the northwest part of the Black Sea and the investigation of the space structure of the field of currents and the role of various factors in its formation.



(a)



(b)



(c)

Fig. 3.6. Intraannual variability of the vertical distributions of temperature T (°C) [(a) 1981, (b) 1983] and salinity S (‰) [(c) 1981] of water computed according to the meteorological data in the one-dimensional version of the model.

Some results of calculations performed for the last decade of May are presented in Figs. 3.7 and 3.8. These calculations were carried out since the second decade of March with assimilation of the data on the air temperature and thermohaline structure on the open sea boundary for the constant wind conditions. The thermohaline stratification on the liquid boundary was specified for each decade according to the data from [14] and the air temperature was specified with intervals of 6 h according to the data obtained in 1994. The averaged discharges of the Dnieper and Yuzhnyi Bug for the analyzed period were set equal to 1520 and $80\ m^3/sec$, respectively.

Among the general regularities, one should especially mention the following facts: In the major part of the water area, the currents observed in the surface layer are directed along the wind (Fig. 3.7a). As an exception, we can mention the zone of the tongue of freshened waters over the Odessa Bank, where the thermohaline component of currents is predominant in spring. For the southeast wind, the thermohaline surface currents in the zone of the tongue of freshened waters compensate the wind currents (Fig. 3.7b) and, thus, the intensity of the resulting circulation of waters is smaller than in the case of action of only the wind component of currents. In the bottom layer of the relatively deep south part of the computational region, the compensating current is formed with the sign of vorticity opposite to the sign of surface circulation (Fig. 3.7h). Note that the contribution of the barotropic component to the total structure of the field of currents is significant due to the morphological specific features of the basin.

The weaker the wind force, the higher the degrees of heating and freshening of the surface layer (Fig. 3.8). The temperature of water in the Dnieper–Bug Firth and the neighboring water area of the sea in April–May is always several degrees higher than in the remaining part of the analyzed region in agreement with the data of observations presented in [14]. The space structure and intensity of the wind component of circulation of waters in the Odessa region of the northwest part of the Black Sea are close to the results obtained in [99] by using an independent model.

The description of the process of propagation of the tongue of freshened waters from the Dnieper–Bug Firth obtained according to the model described above is in good agreement with the data of observations presented in [9]. According to the climatic data of the "Odessa-port" hydrometeorological station [21], the mean levels of salinity of waters in this region in April and May are equal to 12.8 and 11.7‰, respectively, which also agrees with the numerical results obtained in the presence of the southeast wind whose repetition in the spring period is equal to 22–25% (see Fig. 3.8).

In the third series of numerical experiments, we model the process of formation of the thermohaline structure and the variations of the circulation of waters in the spring–summer period (March – August) with assimilation of the data of regular observations over the air temperature and the velocity and direction of the winds performed every 6 h at the "Odessa-port" hydrometeorological station in 1986. The computational region was somewhat extended to the south (72×38 nodes with steps of 2000 m) in order to take into account the freshwater discharge of the River Dniester (Fig. 3.4). According to the numerical results, the discharge of the Dnieper in spring increases from $1300\ m^3/sec$ in March to $3300\ m^3/sec$ in May.

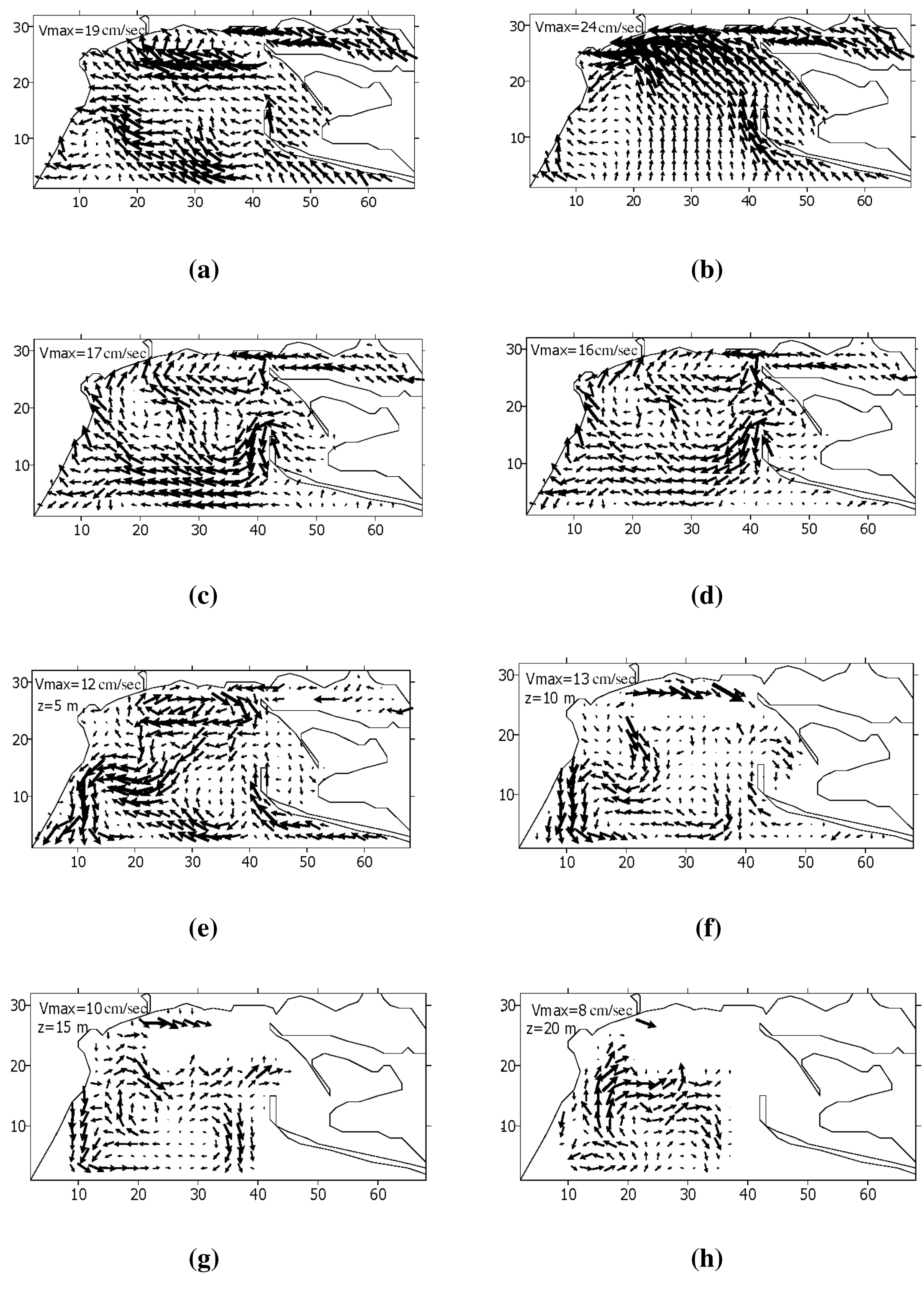
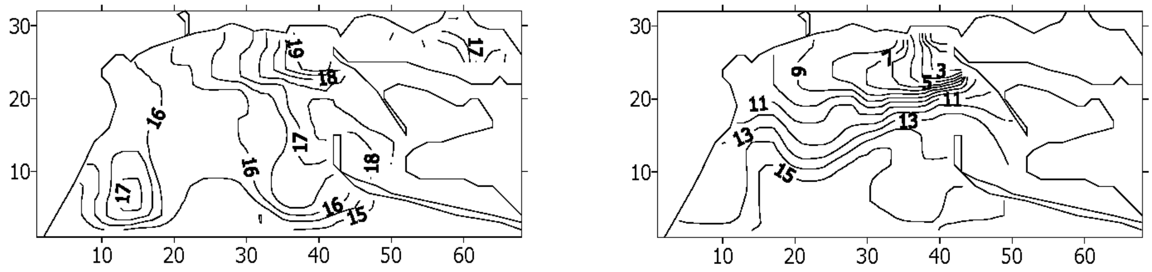
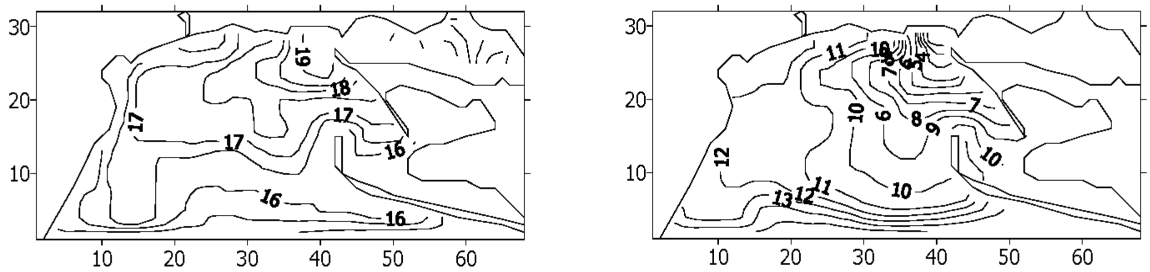


Fig. 3.7. Fields of the vectors of currents computed according to the model for the last decade of May in the surface layer: (a) total currents for the southeast wind with a speed of 7 m/sec, (b) wind currents for the southeast wind with a speed of 7 m/sec; (c) total currents for the southeast wind with a speed of 3 m/sec; (d) thermohaline and discharge currents in the absence of the wind; total currents for the southeast wind with a speed of 7 m/sec at depths of: (e) 5, (f) 10, (g) 15, and (h) 20 m.



(a)



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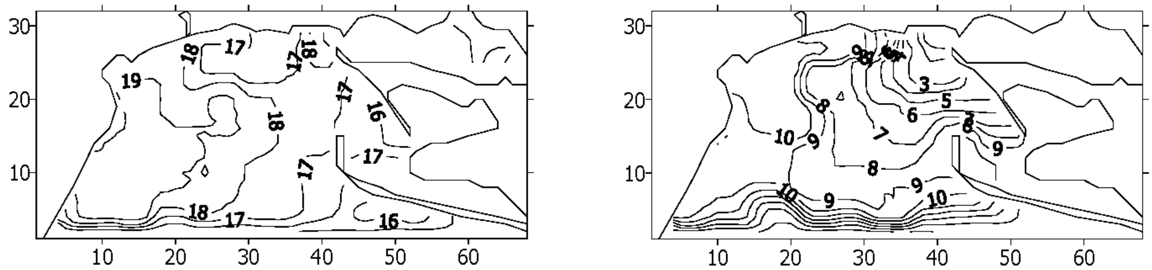


(c)

Fig. 3.8. Distributions of temperature (to the left) and salinity (to the right) of waters in the surface layer computed according the model for the last decade of May in the presence of the southeast wind with the following speeds: (a) 7 m/sec, (b) 3 m/sec, (c) 0m/sec (calm).

The discharge of the Dniester increases from $195\,m^3/sec$ in March to $320\,m^3/sec$ in June. However, the discharge of the Yuzhnyi Bug decreases from $200\,m^3/sec$ in March to $80\,m^3/sec$ in May. Till the end of August, the discharges of all these rivers decrease from the indicated values to 690, 185, and $50\,m^3/sec$ for the Dnieper, Dniester, and Yuzhnyi Bug, respectively.

The results of numerical analysis of the circulation of waters and the distributions of temperature and salinity over the surface layer in the spring–summer period of 1986 are given in Figs. 3.9–3.14. In Fig. 3.15, we present the vertical structure of currents for one day from the period of computations. In order to study the effect of wind conditions on the variations of the thermohaline structure of waters in the investigated water area, we also performed the numerical analysis with assimilation of the daily average values of the data of observations over the winds carried out in 1981 (this year was characterized by the intense wind activity for the entire spring–summer period). In this case, we used the data on the variations of air temperature in 1986. Some results of numerical calculations are presented in Figs. 3.16. 3.17, and 3.18b.

The numerical simulation of the circulation of waters shows that the following picture is typical of the spring period (Fig. 3.9) when the influence of freshwater discharge on the structure of currents in the surface layer is maximum: On leaving the Dnieper–Bug Firth, the current turns to the south following an isobath of 10 m and separates (near the west coast of the Kinburnskaya Spit) into two flows. One of these flows goes to the west along the Odessa Bank, approaches its west slope, and separates into the branch turning to the west along the Dnieper Trough and closing the anticyclonic gyre in the region of the bank and the second branch directed toward Cape Bol'shoi Fontan.

The second flow of the current leaves the Kinburnskii Strait and immediately turns to the south. Then it goes around the north end of the Tendrovskaya Spit, turns to the southwest toward the center of the south boundary of the computational region, and finally, turns to the northwest in the direction of Cape Bol'shoi Fontan. Thus, in the water area of the sea located to the east of Cape Bol'shoi Fontan, we observe the convergence of two currents moving from the northeast and southeast. Further, depending on the predominant winds, the indicated joined current can either move to the south along the west coast or bifurcate into the north and south branches.

The outlined structure of currents is destroyed under the action of strong winds when the wind component of the resulting currents becomes predominant in the entire analyzed water area (Figs. 3.9e and 3.16).

The distribution of salinity over the surface layer in spring is in good agreement with the specific features of the field of surface currents in this period (Fig. 3.11). We detect two tongues of freshened waters propagating from the Dnieper–Bug Firth. The first tongue is better pronounced and directed along the Odessa Bank toward Odessa, whereas the second tongue is directed to the south along the Tendrovskaya Spit. For strong long-term winds with the east component (as, e.g., in spring 1981), the tongue directed toward Odessa becomes predominant and widens up to the Tendrovskaya Spit, thus absorbing, in fact, the south–southwest current of freshened waters (Fig. 3.17). The influence of freshwater discharge of the Dniester is traced only in a local region of the sea near the Dniester Firth.

The river discharge weakens in the summer period of the year. As a result, the contribution of the thermohaline component to the total structure of currents becomes much smaller than in spring. In this period of the year, the wind-induced currents are predominant. Therefore, the stationary eddy structures in the field of surface currents are not traced, their general structure becomes more homogeneous, and the direction of currents is, in general, determined by the direction of the wind (Figs. 3.10 and 3.16). The core of the transformed Dnieper and Yuzhnyi Bug waters is localized within the limits of the east half of the Odessa Bank (Figs. 3.12 and 3.17).

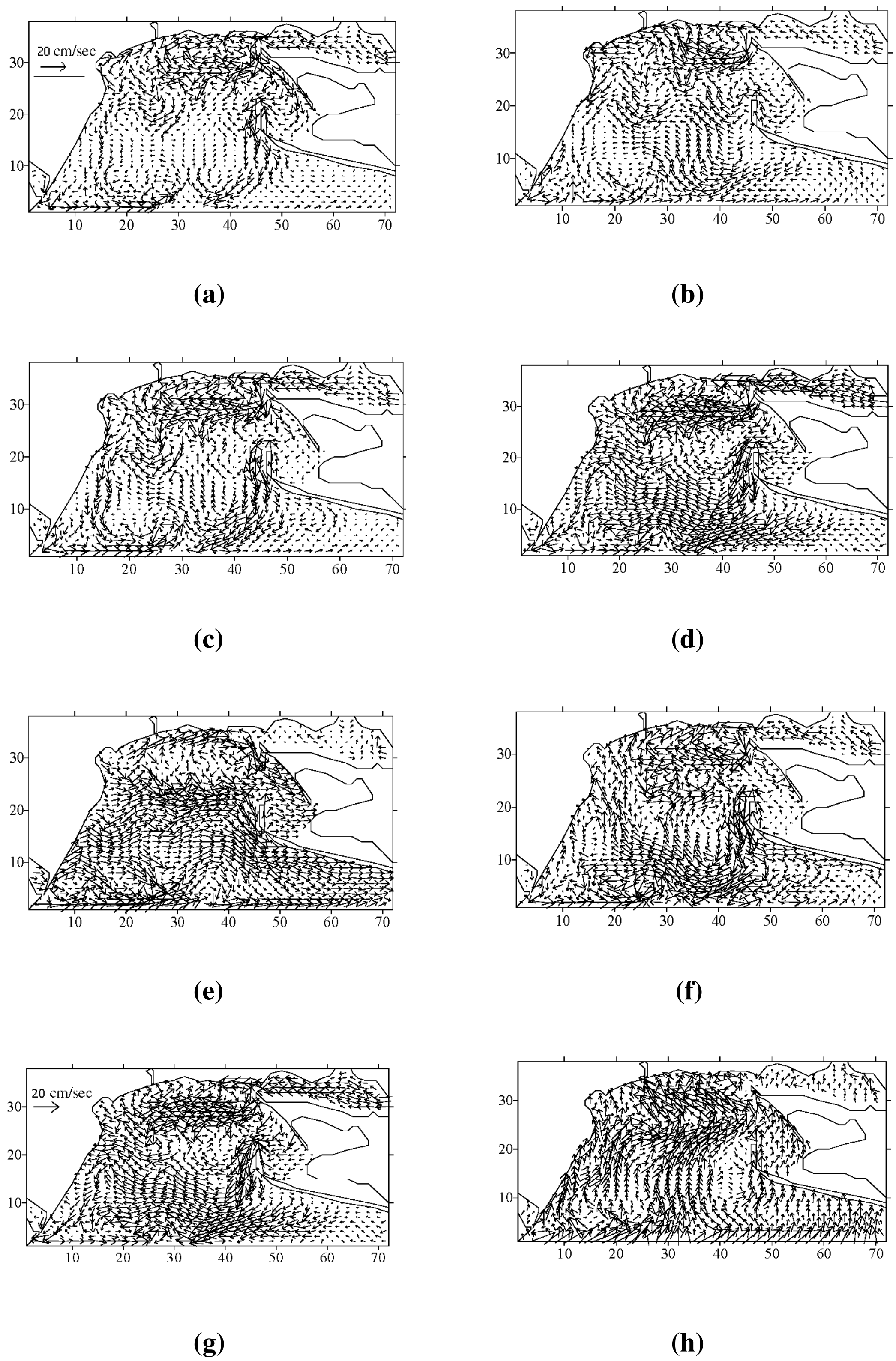


Fig. 3.9. Fields of the vectors of surface currents computed according to the model for the following dates: (a) 10.04.1986, (b) 20.04.1986, (c) 30.04.1986, (d) 10.05.1986, (e) 20.05.1986, (f) 30.05.1986, (g) 10.06.1986, (h) 20.06.1986. The steps of the computational grid $\Delta x = \Delta y = 2000\,\text{m}$.

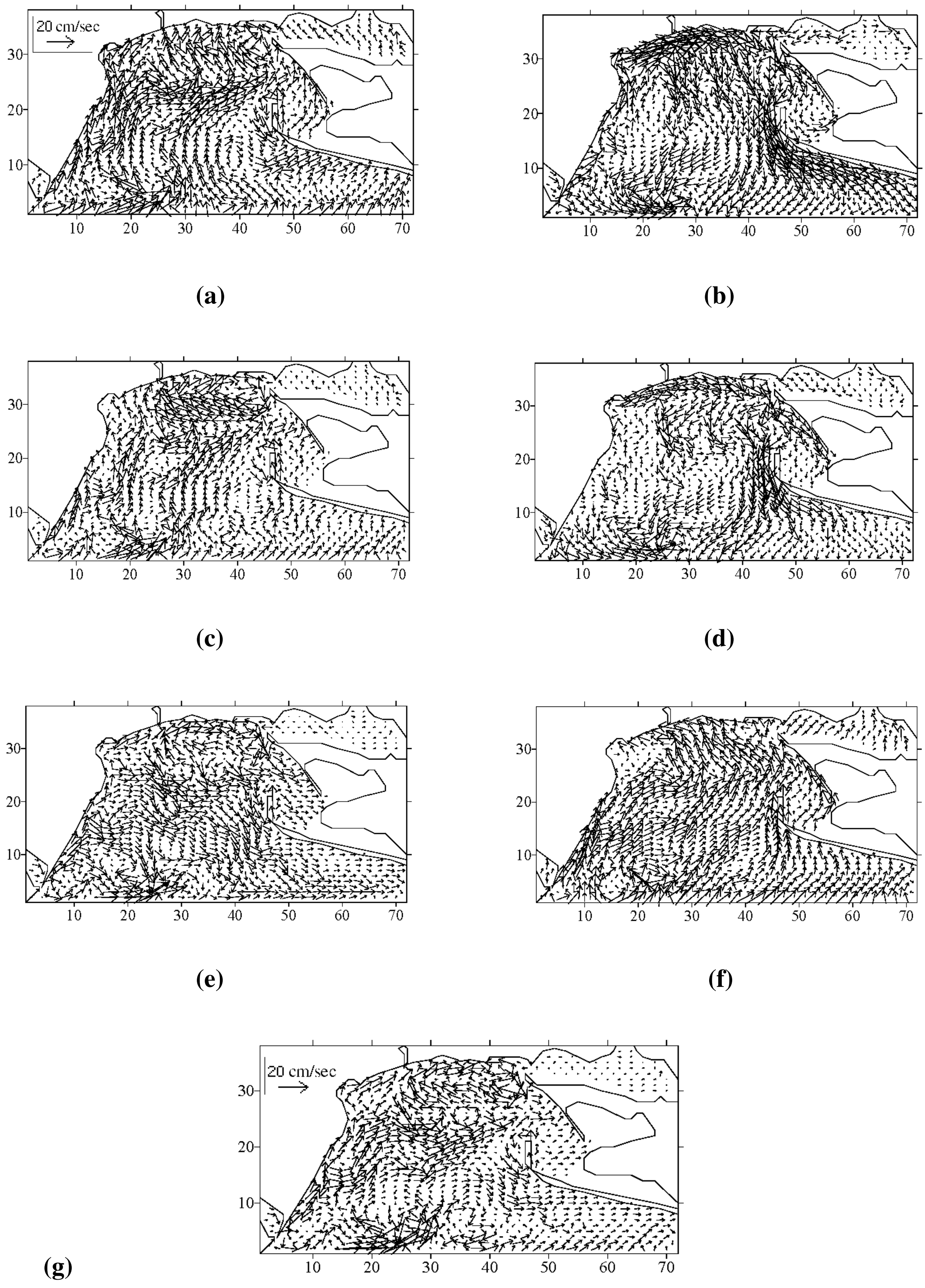


Fig. 3.10. Fields of the vectors of surface currents computed according to the model for the following dates: (a) 30.06.1986, (b) 10.07.1986, (c) 20.07.1986, (d) 30.07.1986, (e) 10.08.1986, (f) 20.08.1986, (g) 30.08.1986.

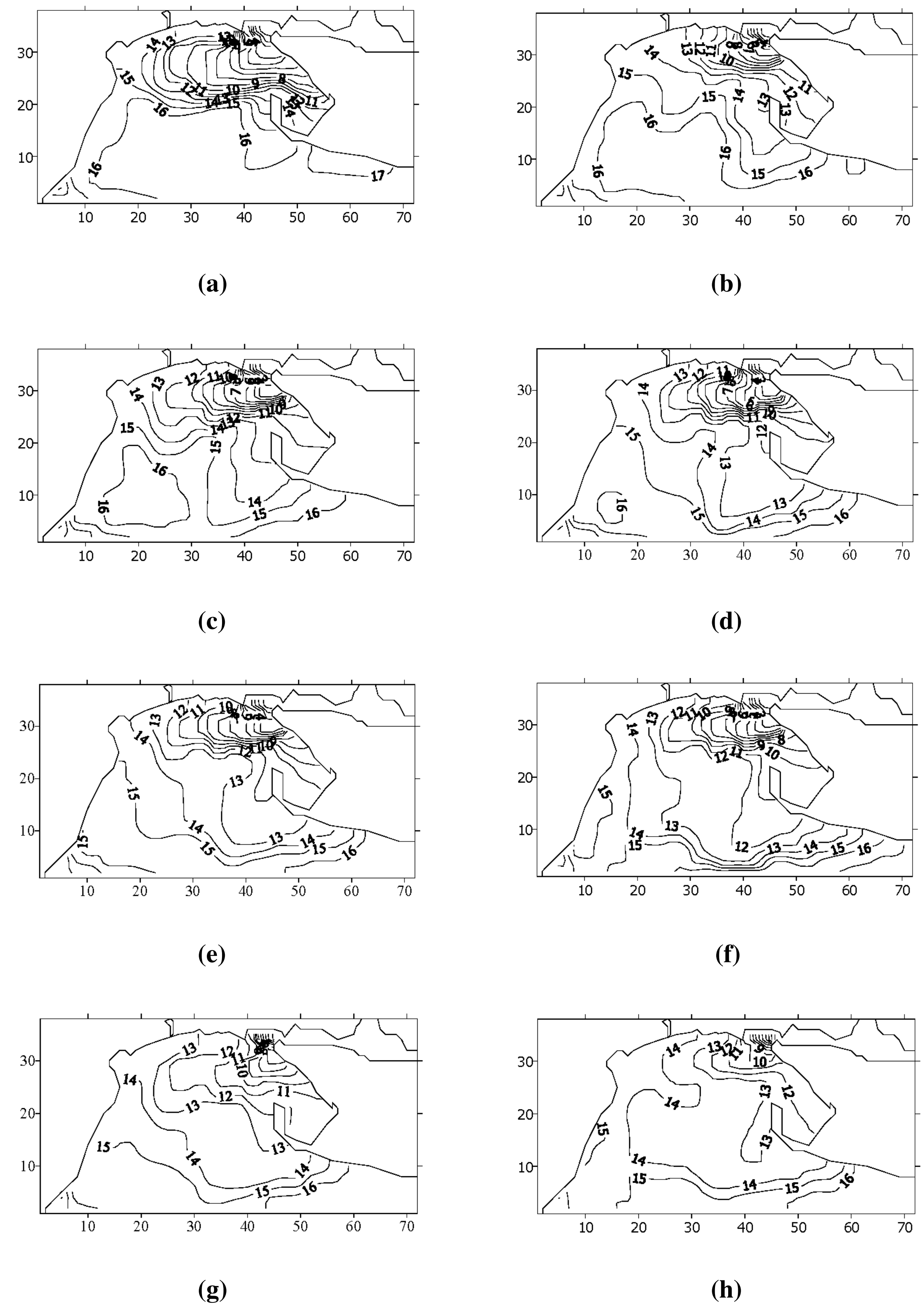


Fig. 3.11. Fields of salinity (‰) of the surface layer of water computed according to the model for the following dates: (a) 10.04.1986, (b) 20.04.1986, (c) 30.04.1986, (d) 10.05.1986, (e) 20.05. 1986, (f) 30.05.1986, (g) 10.06.1986, (h) 20.06.1986.

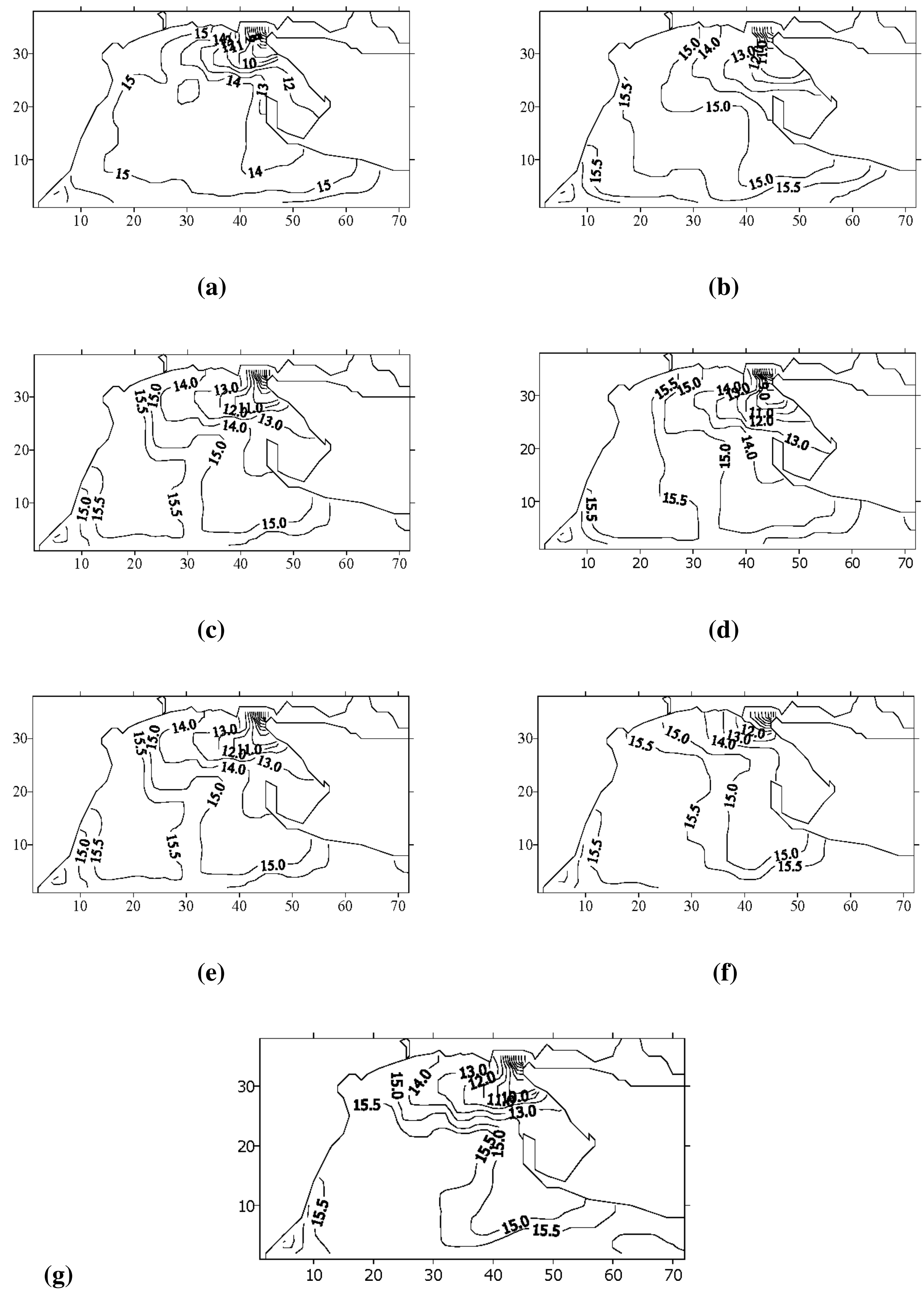


Fig. 3.12. Fields of salinity (‰) of the surface layer of water computed according to the model for the following dates: (a) 30.06.1986, (b) 10.07.1986, (c) 20.07.1986, (d) 30.07.1986, (e) 10.08.1986, (f) 20.08.1986, (g) 30.08.1986.

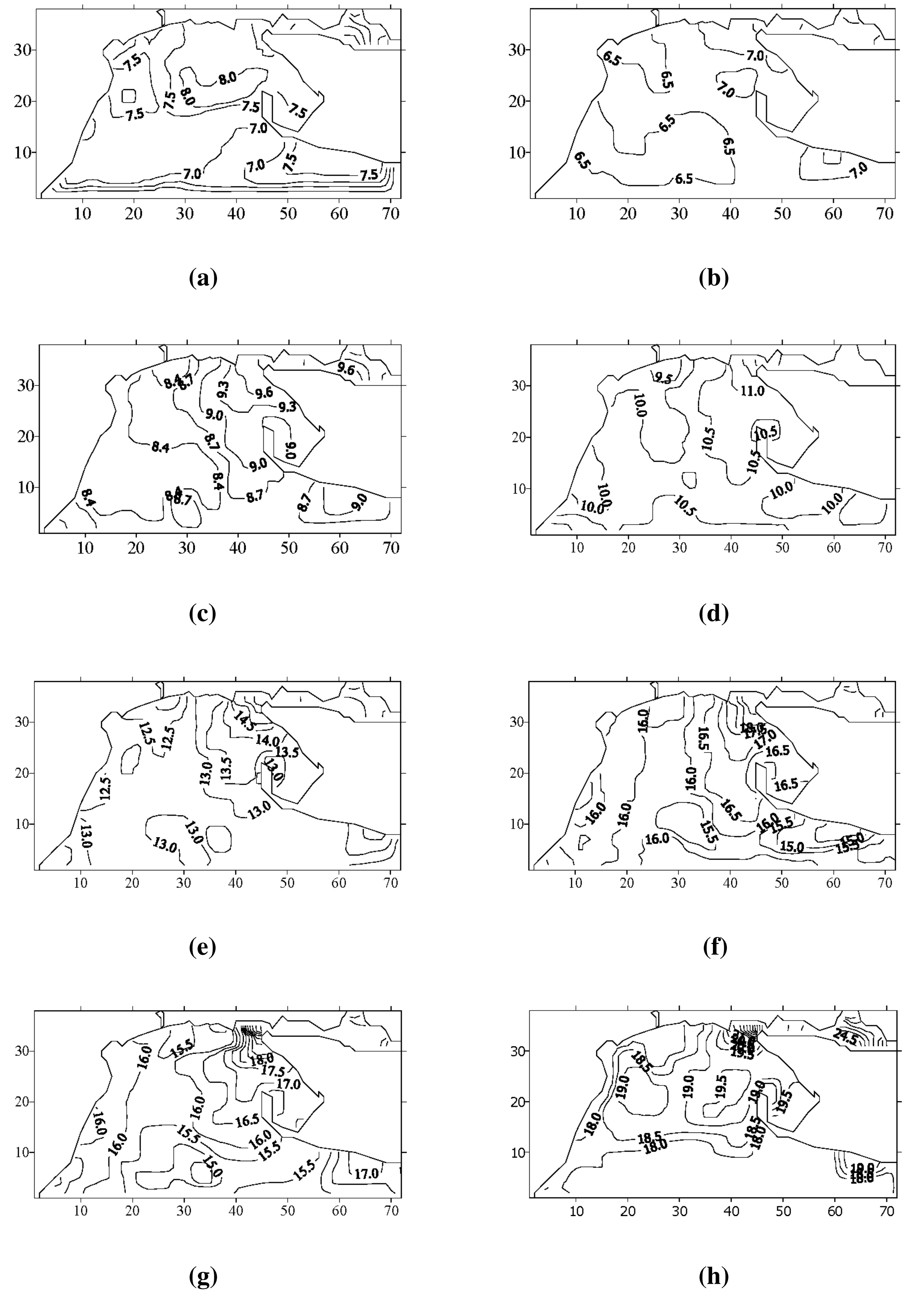


Fig. 3.13. Fields of temperature (℃) of the surface layer of water computed according to the model for the following dates: (a) 10.04.1986, (b) 20.04.1986, (c) 30.04.1986, (d) 10.05.1986, (e) 20.05. 1986, (f) 30.05.1986, (g) 10.06.1986, (h) 20.06.1986.

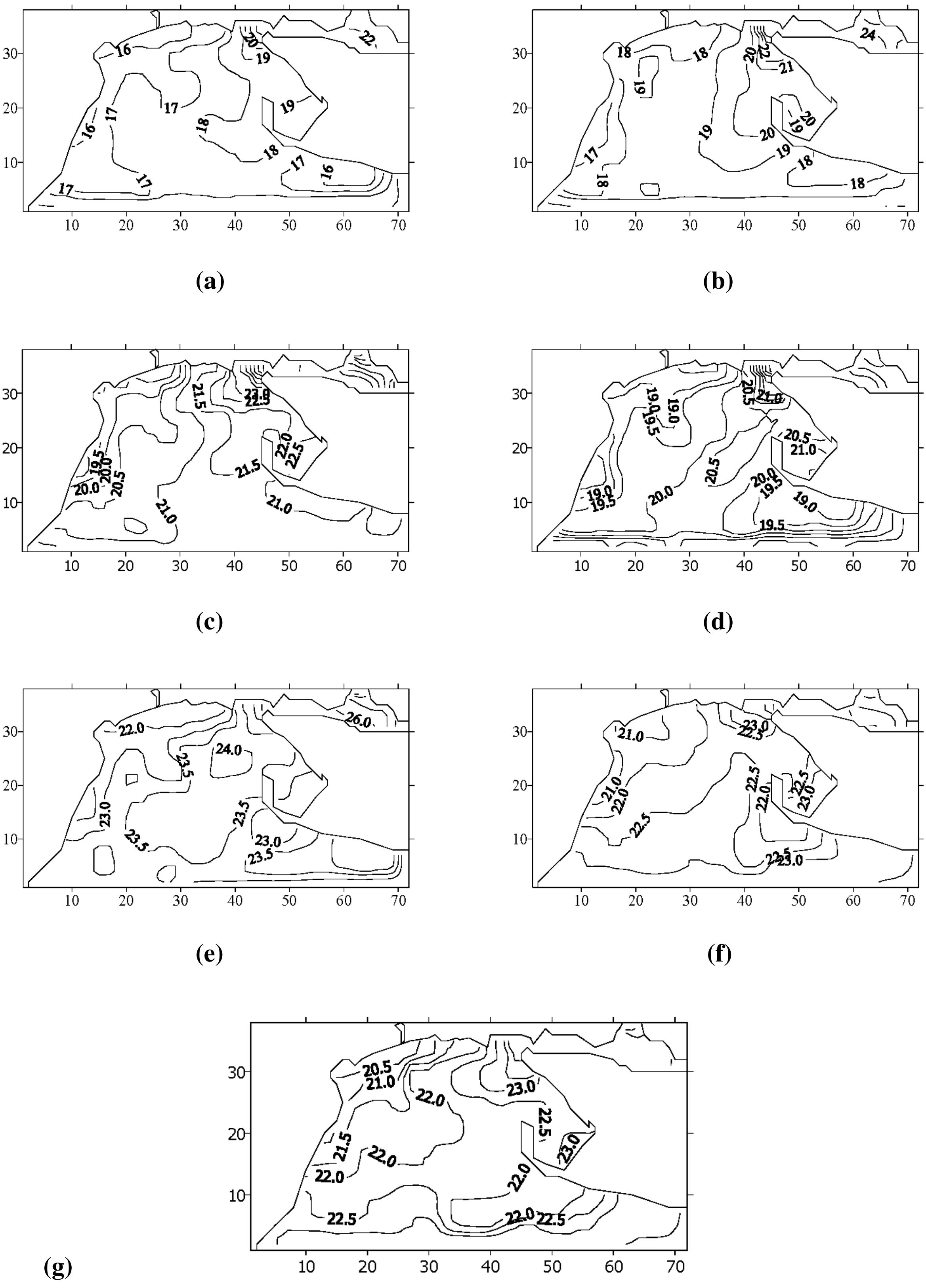


Fig. 3.14. Fields of temperature (℃) of the surface layer of water computed according to the model for the following dates: (a) 30.06.1986, (b) 10.07.1986, (c) 20.07.1986, (d) 30.07.1986, (e) 10.08. 1986, (f) 20.08.1986, (g) 30.08.1986.

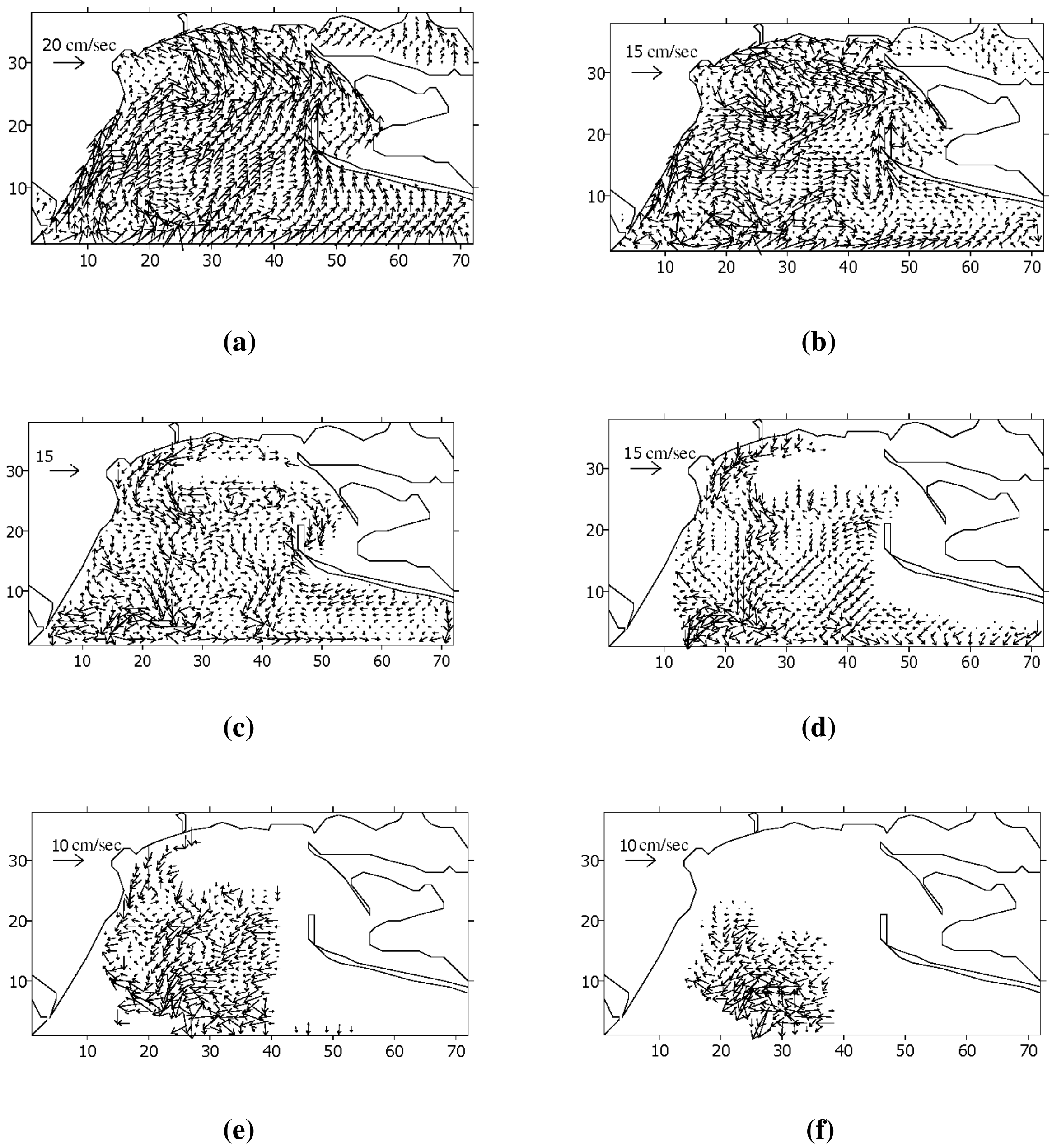


Fig. 3.15. Fields of the vectors of horizontal currents computed according to the model for 20.08.1986 at the following depths: (a) 0 m, (b) 5 m, (c) 10 m, (d) 15 m, (e) 20 m, (f) 25 m.

The results of modeling of the spring–summer heating of the surface water masses and the variability of the space distribution of the surface temperature of water show that the model correctly describes the seasonal course of temperature and the processes of formation and destruction of the seasonal thermocline (Figs. 3.13, 3.14, and 3.18). As follows from these figures, the freshened waters are heated in spring to a greater extent than seawater [14]. In the summer period, the phenomenon of coastal upwelling accompanied by the decrease in the temperature of water in the surface layer of the coastal zone of the sea is observed in the Odessa region of the northwest part of the Black Sea.

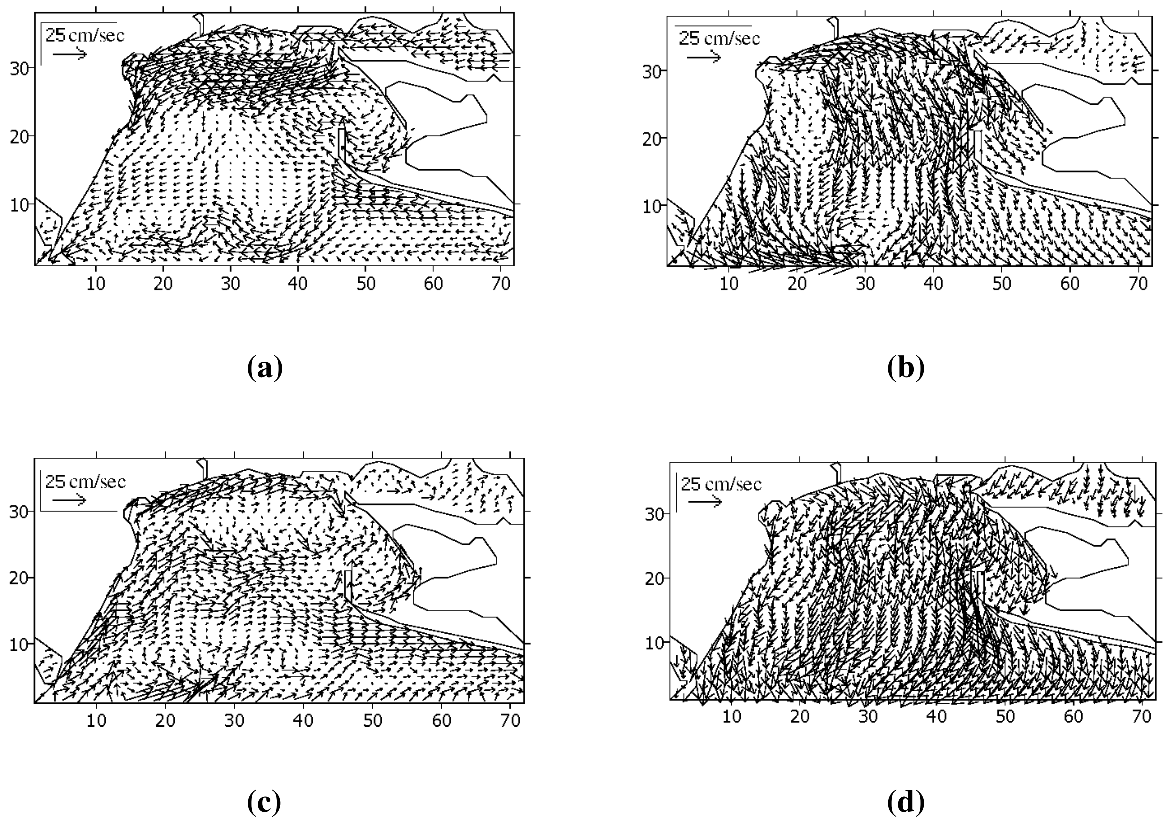
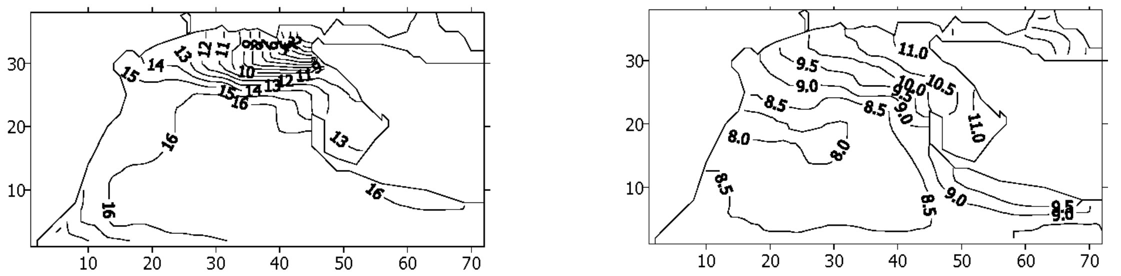


Fig. 3.16. Fields of the vectors of surface currents computed according to the model for the following dates: (a) April 30, (b) May 20, (c) July 20, (d) August 10. The wind conditions reproduce the data of observations carried out in 1981.

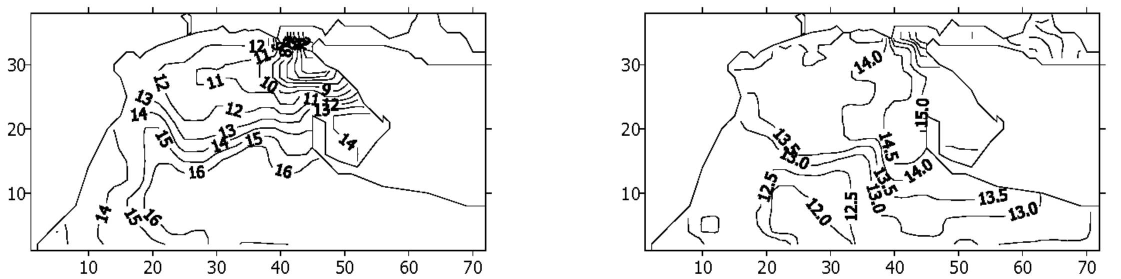
In Fig. 3.18, we illustrate the evolution of the vertical profiles of temperature and salinity in March–August computed according to the proposed model at the point with coordinates $42°23'$ N, $30°53'$ E [node (20; 22) of the computational grid; Fig. 3.4] located in the Odessa region of the northwest part of the Black Sea at a distance of about 16 km from Cape Bol'shoi Fontan in the direction of the open sea. It should be emphasized that the upper mixed layer is formed in the summer period. The depth of the lower boundary of the upper mixed layer varies from 5 to 10 m depending on the wind force. In the bottom layer, the temperature of water increases in the analyzed period from 4 to 12°C. At the same time, the surface temperature increases from 4 to 22°C in agreement with the data of *in-situ* observations [14, 34].

Conclusions

The hydrodynamic block of the model of the quality of waters in shelf ecosystems is, in fact, a three-dimensional prognostic hydrodynamic model realized in a coordinate system curvilinear in the vertical direction by using implicit finite-difference schemes.



(a)



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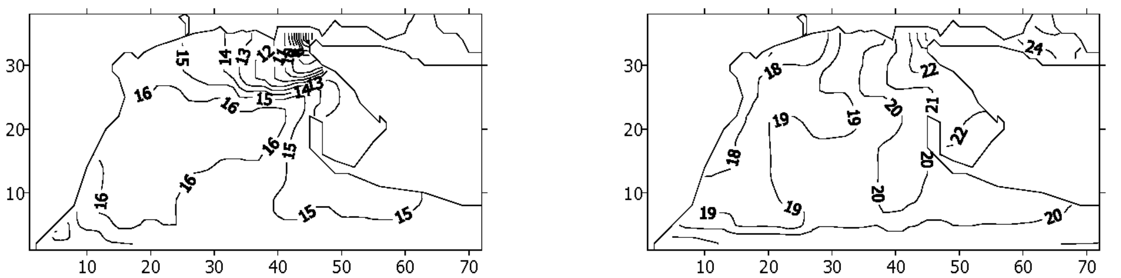

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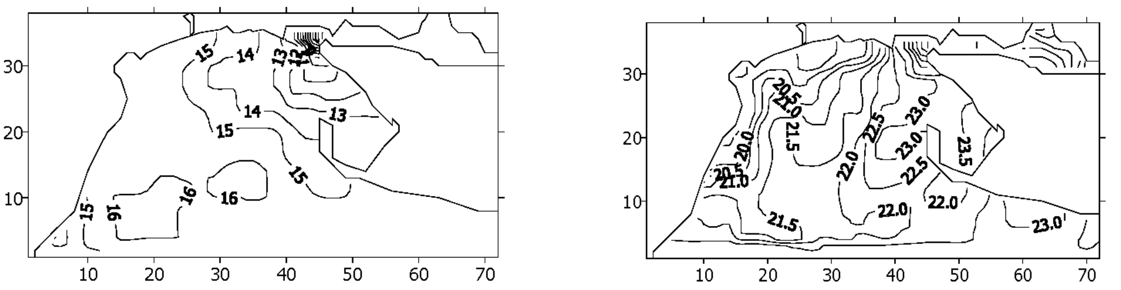
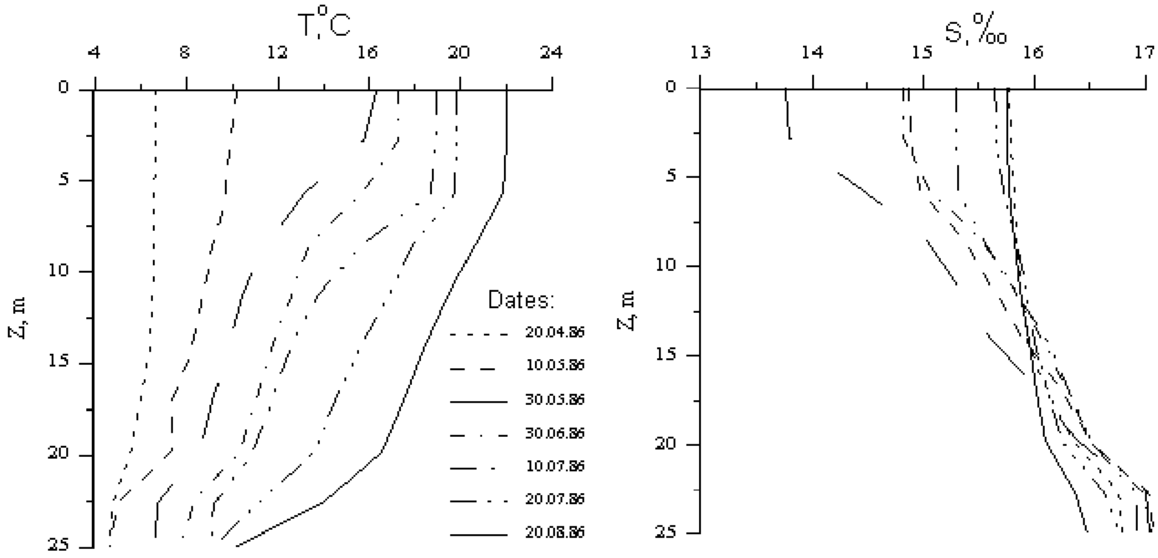
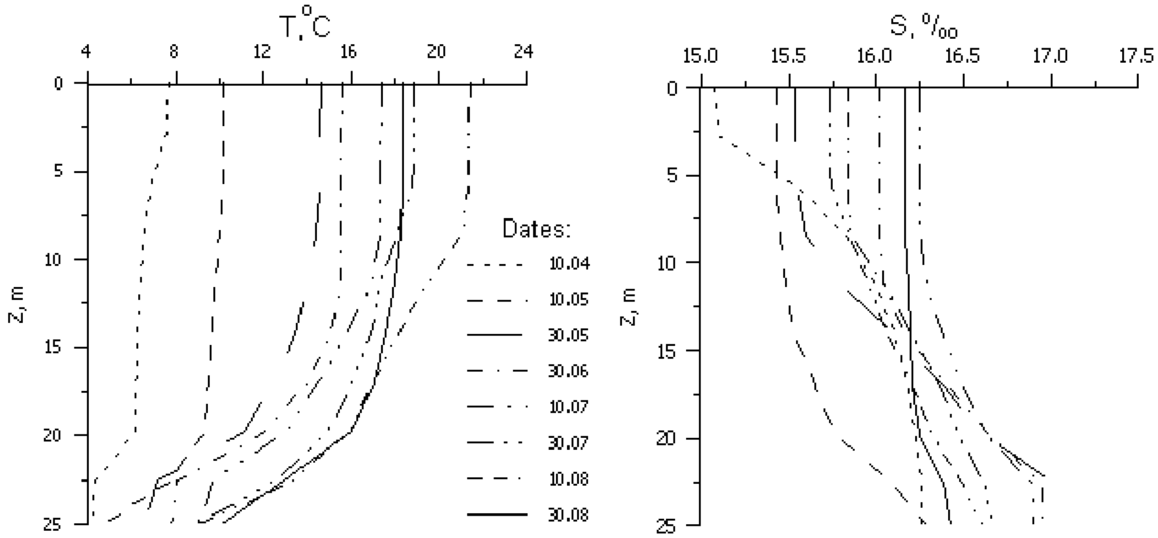


(d)

Fig. 3.17. Fields of salinity (to the left) and temperature (to the right) in the surface layer of waters computed according to the model for the following dates: (a) April 30, (b) May 20, (c) July 20, (d) August 10. The air temperature and wind conditions correspond to the data of observations carried out in 1986 and 1981, respectively.



(a)



(b)

Fig. 3.18. Variations of the vertical distributions of temperature (to the left) and salinity (to the right) of waters at node (20; 22) according to the results of numerical analysis performed with assimilation of the meteorological data of the "Odessa" hydrometeorological station: (a) air temperature and wind conditions are specified according to the data of observations for 1986; (b) air temperature and wind conditions are are specified according to the data of observations for 1986 and 1981, respectively. The displayed curves correspond to the indicated dates in the spring–summer period (March–August).

The model is equipped with a block of assimilation of hydrometeorological data on the boundaries of the analyzed region and enables one to reproduce the space-time variations of the thermohaline structure of waters, the fields of admixtures, the three-dimensional field of currents, and the intensity of turbulent exchange in water areas of the sea shelf with complex morphological and hydrological characteristics for time intervals from several days to the annual cycle. There exists a possibility to separate the wind, thermohaline, tidal, and discharge components of the total currents by means of operative changes in the number of analyzed factors performed by using control keys. In the proposed model, the analysis of the thermohaline structure of waters can be realized both in the prognostic and diagnostic modes.

The mathematical structure of the model enables us to use it for the shelf areas of the sea some regions of which have subgrid scales in one of the horizontal directions (estuaries of rivers, narrow straits, channels, etc.) and significant areas are covered by the shallow-water basins and the zone of continental slope.

The basic hydrodynamic model is supplemented with a block of transfer of admixtures capable of simultaneous description of the process of propagation of up to 15 nonconservative elements with different properties in a three-dimensional space.

The presented results of numerical analyses of the evolution of thermohaline structure and circulation of waters in the Dnieper–Bug-estuary and Odessa regions in the northwest part of the Black Sea in the spring–summer period carried out according to the proposed hydrodynamic model show that the model adequately reproduces the specific features of variations of the thermohaline structure and circulation of waters in the investigated water area.

The indicated computational possibilities of the hydrodynamic model enable us to use it as the basic hydrodynamic block of the model of quality of waters in the shelf ecosystems of the sea.

4. MATHEMATICAL STRUCTURE OF THE CHEMICAL-AND-BIOLOGICAL BLOCK OF THE MODEL OF QUALITY OF WATERS

The chemical-and-biological block of the analyzed model of the quality of waters in the shelf ecosystems of the sea is formed by the following two parts:

— the block of self-cleaning used to determine the decreasing concentration of pollutants at every local point of the space with regard for the combined action of various physicochemical, chemical, biochemical, and biological processes running in marine media;

— the block of eutrophication in the form of a system of coupled differential equations aimed at the description of the biogeochemical cycles of biogenic elements, production and destruction of the organic substances, trophic links, and the dynamics of oxygen at any local point of the marine medium.

In fact, the block of self-cleaning can be described as a family of functional dependences specifying the rates of the processes of degradation and destruction of pollutants in marine media.

The block of eutrophication has a more complicated mathematical structure because, in fact, it can be regarded as a model of functioning of water ecosystems with high levels of aggregation of the biotic components. This block describes the direct and inverse relations between the biotic and abiotic elements of the ecosystem under the necessary condition of validity of the laws of conservation of matter and energy.

Even if the general principles of construction are preserved, the specific mathematical structure and complexity of the block of eutrophication of the model of the quality of waters developed for the investigated water area of the sea have their own individual distinctive features caused by the morphological characteristics of the basin, specific character of the formation of hydrological and hydrochemical modes of waters, and, in many cases, the degree of completeness of the data of monitoring of the typical values and variations of the modeled parameters of the quality of waters and the natural and anthropogenic factors affecting these parameters. Therefore, the models of eutrophication developed and applied for various water areas of the sea can differ both by the number of variables of state of the ecosystem taken into account by the model and the degree of going into detail in the description of some chemical and biological processes.

In this chapter, we present a detailed description of the mathematical structure of the blocks (models) of eutrophication developed by the authors for various marine basins of the Caribbean coast of Colombia and the Dnieper–Bug estuary region in the northwest part of the Black Sea. The application of each of these blocks imposes its own requirements on the initial data accumulated in the course of realization of the ecological monitoring of modeled objects. Moreover, the application of eutrophication blocks of different degrees of complexity and organization is explained by the necessity of taking into account the specific features of formation of the quality of waters in the investigated water areas of the sea and the levels of their trophicity, saprobity, and bioproductivity.

Thus, the models of eutrophication developed for the tropical water basins of the Caribbean coast of Colombia do not take into account the influence of the temperature of water on the rate of chemical and biological processes because the annual variations of temperature do not exceed 3–5°C and their amplitude is comparable with the amplitude of diurnal oscillations. At the same time, the time step used in these models is set equal to 1 h because the influence of tidal oscillations of the sea level on the space and time variations of modeled parameters is significant. The inert organic matter was not separated into the organic compounds of nitrogen and phosphorus because their concentrations were not determined in the course of ecological monitoring due to the methodical problems. However, the results of special experiments performed somewhat later show that the rates of regeneration of the mineral compounds of nitrogen and phosphorus are identical under the conditions typical of the investigated tropical water areas of the sea [127].

On the contrary, the analysis of the data of hydrochemical monitoring in the Odessa region of the northwest part of the Black Sea shows that the difference between the rates of mineralization of organic nitrogen and phosphorus and the ratio of nitrogen and phosphorus in the compositions of allochthonous and autochthonous organic matter in waters of the investigated water area can be significant [86]. In order to study these specific features, the phosphorus and nitrogen cycles are separated in the model of eutrophication.

The methodology and results of application of the proposed models of the quality of waters to the solution of practical problems aimed at the preservation and improvement of the ecological state of open and closed water areas in the shelf zone of the sea are discussed in Chapter 7.

4.1. Block of Self-Cleaning of Waters From Pollutants of the Anthropogenic Origin

The problem of self-cleaning of waters in the investigated water area of the sea from pollutants of the anthropogenic origin is correct in the case of local character of the source of pollution and in the absence of significant natural sources of pollutants in the water medium. The first condition means that the influence of the source of pollution on the quality of waters and the process of functioning of the ecosystem can be detected only in a local region whose dimensions are much smaller than the size of the investigated region of the sea. As examples of pollutants satisfying the second condition, one can mention oil and oil products, synthetic surfactants, phenols, heavy metals, and other toxicants. Penetrating into marine media, these substances participate in various physical, chemical, biological, and mixed processes resulting either in their transformation into passive (relative to the biotic components of the ecosystem) chemical elements and compounds or their removal from the water medium. This type of pollutants includes biological pollutants especially dangerous for human beings, i.e., the pathogenic bacteria suffering biodegradation in marine media.

Thus, the problem of self-cleaning of waters takes into account solely the natural processes leading to the diffusion, destruction, and transformation of pollutants in the water medium of the investigated water area of the sea or to the removal of these substances from the analyzed region. As a rule, the secondary sources of pollutants in water media are neglected in solving the problem of self-cleaning. In this case, it is assumed either that these sources are absent or that their intensity is much smaller than the intensity of the processes of degradation and decay.

As basic mechanisms of self-cleaning of waters in the investigated water area from the pollutants of toxic action, we can mention the following processes:

— hydrodynamic processes: the processes of dilution of pollutants as a result of convective mixing, advective transfer, and turbulent diffusion;

— physicochemical processes: the processes of removal of pollutants from the bulk of water as a result of their sorption by bottom sediments or particles of the suspension with subsequent gravitational sedimentation of these particles to the bottom, the process of formation of difficultly soluble and complex compounds, the process of liberation of gases from water, etc.;

— chemical processes: the processes of chemical oxidation (realized without participation of molecular oxygen) and photochemical oxidation;

— biochemical processes: the processes oxidation of organic substances and nitrification running with the participation of bacteria;

— biological processes: the processes of removal of pollutants from the bulk of water as a result of their absorption by hydrobionts, bioaccumulation, and subsequent biosedimentation of dead organisms.

The hydrodynamic processes leading to the dilution of polluted waters are regarded as one of the mechanisms of self-cleaning of waters only in a sense that they promote the decrease in the concentration of pollutants to levels lower than the maximum permissible concentrations for waters of the investigated region. The processes of biosedimentation and sorption of pollutants by the suspension and bottom sediments remove pollutants from the bulk of water but create secondary sources of pollution. Thus, the essence of the notion “self-cleaning of waters” is most completely reflected by the processes of chemical and biological nature described in the block with the corresponding name.

The role of various factors in the process of self-cleaning of natural waters depends on the chemical nature of discharged substances, the biomass of microorganisms, their functional activity, the oxygen, temperature, and hydrochemical conditions (e.g., the pH values), the compositions of suspended substances and bottom sediments, and other factors.

It is known that the chemical, biological, biochemical, and physicochemical processes of decay of pollutants under the conditions of water media are closely correlated and run simultaneously. Thus, from the practical point of view, it is reasonable to determine and use the total rates of transformation (nonconservative factors) of pollutants determined either under the *in-situ* conditions or under the laboratory conditions as close to the *in-situ* conditions as possible. In this case, the differential quantitative analysis of separate processes is not realized.

Thus, in constructing the block of self-cleaning of waters from nonconservative pollutants and pathogenic microorganisms, we can assume that the process of destruction of pollutants in aqueous media is described by the following kinetic equation of the first-order reaction:

$$F_i = \left.\frac{dC_i}{dt}\right|_{\text{loc}} = -K_{ci} C_i, \tag{4.1}$$

where F_i is the function of nonconservativeness of an admixture from Eq. (1.1) and K_{ci} is the nonconservative (destruction) factor of the pollutant equal to the specific rate of its transformation under the combined action of physicochemical, chemical, biological, and biochemical processes (without specifying their contributions explicitly).

Thus, the coefficient K_{ci} in Eq. (4.1) plays the role of the integral factor for the processes of chemical and biological nature and is a function of the properties of aqueous media (temperature, salinity of water, pH value, etc.). Its values for specific types of pollutants can either be taken from the literature or found empirically by using dependences of the form

$$K_{ci} = \frac{1}{t - t'} \ln \frac{C_i^0}{C_i^t} \tag{4.2}$$

or

$$K_{ci} = \frac{\ln 2}{\tau_i}, \tag{4.3}$$

where C_i^0 is the initial concentration of the ith pollutant, C_i^t is its concentration at time t, t' is a period of time for which the concentration C_i^0 remains practically constant (the period of adaptation of microorganisms), and τ_i is the half-life period of the ith substance.

At present, sufficiently detailed data on the mechanisms and rates of destruction of various groups of harmful organic substances (such as phenols, synthetic surfactants, oil products, chlororganic compounds, etc.) accumulated in the course of various special experiments carried out by numerous researchers are available from the literature [82, 84].

Generally speaking, the applicability of the first-order kinetic equation to the description of the processes of destruction of pollutants in marine media means that there exists a linear dependence of the logarithm of concentration of the analyzed pollutant $\log C_i(t)$ on time t.

In some cases, the required data are available and the destruction factor K_{ci} can be represented in the multiplicative form as a function of the parameters of ambient medium specifying this quantity. Thus, the process of biodegradation of pathogenic microorganisms of the *E. coli* group (Coliforms) in seawater is described by the following formula [144, 146]:

$$K_c^{\text{coli}} = \begin{cases} k_n \lambda_S^{(S)} \lambda_T^{(T-20)} & \text{at night,} \\ \max\left(k_n \lambda_S^{(S)} \lambda_T^{T-20}, \dfrac{k_l}{\alpha H}(1 - \exp(-\alpha H)) \right) & \text{during the daytime,} \end{cases} \tag{4.4}$$

where k_n is the death rate of Coliforms at night for the temperature of water $T = 20°\text{C}$ and the level of salinity $S = 0‰$ ($k_n \approx 0.8\ \text{day}^{-1} \approx 0.033\ \text{h}^{-1}$), $\lambda_S^{(S)}$ and $\lambda_T^{(T-20)}$ are the correction coefficients for the *in-situ* thermohaline conditions, where $\lambda_S = 1.006$ and $\lambda_T = 1.07$, and k_l is the experimentally determined mean death rate of the Coliforms in the surface layer of water during the daytime.

One of the most important mechanisms of self-cleaning of seawater from heavy metals is their sorption by particles of the suspension with subsequent gravitational sedimentation to the bottom. The process of mass exchange between the dissolved and suspended (i.e., sorbed by suspended particles) fractions of a pollutant is described by the following equation [38]:

$$Q_{\text{sus-w}}^{\text{sorb}} = \nu_{\text{sus-w}} S_{\text{sed}} (k_d C - C_{\text{sus}}), \tag{4.5}$$

where $Q_{\text{sus-w}}^{\text{sorb}}$ is the sorption–desorption flux of the pollutant in the water–suspension system, $\text{mg/m}^3 \cdot \text{day}$, $\nu_{\text{sus-w}}$ is a constant characterizing the intensity of sorption exchange in the water–suspension system, day^{-1}, k_d is the coefficient of equilibrium distribution for the indicated system according to the Henry law, C is the concentration of pollutant in seawater in the dissolved form, mg/m^3, C_{sus} is the concentration of pollutant (POL) adsorbed by suspended particles (SUS) (suspended fraction), mg(POL)/mg(SUS), and S_{sed} is the concentration of suspension in seawater, mg/m^3.

In the processes of monitoring and numerical analysis, it is necessary to distinguish the dissolved and suspended (adsorbed by particles of the suspension) fractions of the pollutant. Unlike the dissolved fraction, the suspended fraction is characterized by a nonzero velocity of gravitational sedimentation depending on the density and sizes of suspended particles. For particles of the suspension whose sizes do not exceed $0.5\ \text{mm}$, this velocity can be estimated according to Stokes' law as follows:

$$w_g = \frac{gd^2(\rho_s - \rho_w)}{18\mu\rho_w}, \tag{4.6}$$

where ρ_s and ρ_w are, respectively, the densities of suspension and seawater, d is the diameter of suspended particles, μ is the dynamic viscosity coefficient of water, and g is the gravitational acceleration. The mass exchange between the suspended and dissolved fractions of the pollutant is described by relation (4.5).

The biodestruction of organic pollutants (e.g., of oil and chlorinated hydrocarbons) runs with active participation of bacteria. In the case where the biomass of bacteria undergoes significant changes inside the analyzed water area or in the course of the process, its mathematical description can be realized by using the following second-order kinetic equation (in the form proposed by Monod):

$$F_i = \frac{dC_i^{\text{org}}}{dt} = -V_b^m \frac{C_i^{\text{org}} B_b}{E(\Pi_i^{\text{org}} + C_i^{\text{org}})}, \tag{4.7}$$

where C_i^{org} is the concentration of the ith organic pollutant, t is time, B_b is the biomass of bacteria, V_b^{opt} is the specific rate of growth of bacteria under the conditions of sufficient supply of the organic substrate, E is the (economic) yield factor characterizing the changes in the biomass of bacteria as a function of the concentration of substrate C_i^{org}

$$\left(E = \frac{dB_b}{dC_i^{\text{org}}} \approx \text{const}\right),$$

and Π_{ci} is the semisaturation constant equal to the concentration of substrate for which $V_b = 0.5\,V_b^m$.

Equation (4.7) contains the biomass of bacteria which, in turn, is a function of the concentration of the organic substrate and the functional characteristics of bacteria. In the simplest case, the dynamics of the biomass of bacteria at every point of the space can be described by a differential equation of the form

$$\frac{dB_b}{dt} = V_b^m \frac{C_i^{\text{org}} B_b}{\Pi_i^{\text{org}} + C_i^{\text{org}}} - \mu_b B_b, \tag{4.8}$$

where μ_b is the specific death rate of bacteria.

Equations (4.7) and (4.8) form a closed system describing the process of biodestruction of the organic substrate with participation of bacteria. Hence, the use of the second-order kinetic equation [taking into account the dependence of the rate of destruction of pollutants on the biomass (concentration) of any element of the ecosystem in the chemical-and-biological block of self-cleaning of waters requires the description of the space and time dynamics of these elements in the model.

In getting the expert estimates, the use of the block of self-cleaning in the model of the quality of waters is reasonable in the cases where it is necessary to determine the dimensions of the zone in which the level of pollution caused by functioning of one or several local sources of pollution exceeds the maximum permissible concentration, to estimate the possibility of exceeding the permissible level of pollution at a certain point (or in a given region) of the water basin for various hydrometeorological conditions and the characteristics of discharge of polluted waters from the sources, and to evaluate the contributions of various local sources to the formation of the level of pollution at a certain point (in a given region) of the water area with an aim to normalize their discharges, etc.

To complete our analysis of the problem of self-cleaning of waters from pollutants, we note that the requirement of locality of the source of pollution as a condition of correctness of the analyzed problem is of especial importance in analyzing the quasiconservative pollutants (stable under chemical and biological transformations) when the process of hydrodynamic dilution as a result of mixing of polluted waters with relatively pure seawater plays the role of the main process of cleaning of waters.

4.2. Block of Eutrophication and the Oxygen Conditions of Waters

As elements of this block, we consider the parameters of the quality of waters in marine ecosystems characterizing the levels of their trophicity and saprobity. As these parameters, we can use the concentrations of mineral compounds of biogenic elements, the biomasses of phytoplankton and bacteria, the concentration of inert organic matter, the oxygen content of waters, and the biochemical oxygen demand (BOD and BOD_5).

The number of equations (1.1) in the block of eutrophication must be equal to the number of variables of a state of the ecosystem specifying the quality of waters, i.e., the mathematical system must be closed.

In the mathematical structure of the block of eutrophication, the main difficulties are encountered in analyzing the role of bacteria in the processes of biochemical oxidation of organic substances, nitrification, and denitrification. The problem is connected with the fact that these processes run with participation of different groups of bacteria whose separate quantitative analysis is methodologically difficult and significantly increases the cost of ecological monitoring of the water ecosystem. In addition, the explicit appearance of all groups of bacteria in the balance equations substantially increases the number of variables of the model and, hence, leads to significant computational difficulties in the processes of calibration, verification, and application of the model. In view of the fact that the data on variations of the biomasses and functional characteristics of these groups of bacteria obtained in the course of monitoring are fairly inaccurate, we have all reasons to expect that the results of model calculations would be random and inadequate to the original. Therefore, in the major part of applied models of eutrophication [5, 18, 80, 118, 128, 129], the rates of the indicated processes are parametrized by the kinetic equation of the first-order reaction, i.e., the influence of the variations of the biomass of bacteria on the rate of the analyzed process is neglected.

However, we can also mention some positive features of the introduction of bacterioplankton in the structure of a model as one of its variables: first, it becomes possible to describe the variations of one of the most significant pools of organic matter in the water ecosystem (and, hence, to give, as a final result, a more exact description of the dynamics of all elements of the ecosystem and the quality of its waters as a whole) and, second, in the case where the analyzed water basin contains powerful sources of allochthonous organic matter and, therefore, is characterized by significant spatial inhomogeneities of the concentration of inert organic matter, the analysis of the role of bacterioplankton enables us to give a more adequate picture of the space and time variations of the flux of biogenic elements regenerated in the process of mineralization of organic matter. Note that this flux, to a significant extent, determines the level of trophicity of waters. Thus, there exists a fairly long list of models [32, 49, 65, 134, 166] in which bacterioplankton is regarded as one of the key biotic elements of the ecosystem responsible for the quality of its waters. In this case, the process of mineralization of organic matter is described by the second-order kinetic equation.

The mathematical structure of the block of eutrophication of the model of the quality of waters for a given aqueous object largely depends on the specific character of posed problems and the completeness of the source data about the object accumulated in the course of ecological monitoring. On the one hand, the model must adequately reproduce the variations of the characteristics of natural analog specified by the purposes of simulation and, on the other hand, it must require the minimum possible amount of the initial data for the purposes of adaptation, calibration, and verification or should be based on the initial data obtained earlier (often for the other purposes). Since complex ecological studies of the sea require significant costs, the role played by the economic factors in the choice of the type of the model and its developer often becomes decisive. Therefore, in what follows, we present the description of the mathematical structure of four different versions of the block of eutrophication. Each of these blocks was successfully used for the solution of the posed applied problem for a specific water basin and, at the same time, required reasonable (in the financial and methodical aspects) volume of the initial data.

4.2.1. Simple Block of Eutrophication for a Shallow-Water Tropical Water Basin Suffering Powerful Anthropogenic Loads

The proposed version of the block of eutrophication includes seven basic ecosystem elements characterizing the utilization and regeneration of the mineral compounds of biogenic elements in the ecosystem and the oxygen conditions of the water basin: phytoplankton B_f, labile inert organic matter B_{org}, phosphates C_{PO_4}, ammonium C_{NH_4}, nitrites C_{NO_2}, nitrates C_{NO_3}, and dissolved oxygen C_{O_2}. The block diagram of the model is presented in Fig. 4.1.

In constructing the mathematical structure of the block of eutrophication, it is assumed that the cycles of nitrogen and phosphorus in the biotic component of the ecosystem are closed on the level of phytoplankton and the processes of regeneration of their mineral compounds are satisfactorily described by the kinetic equation of the first-order reaction.

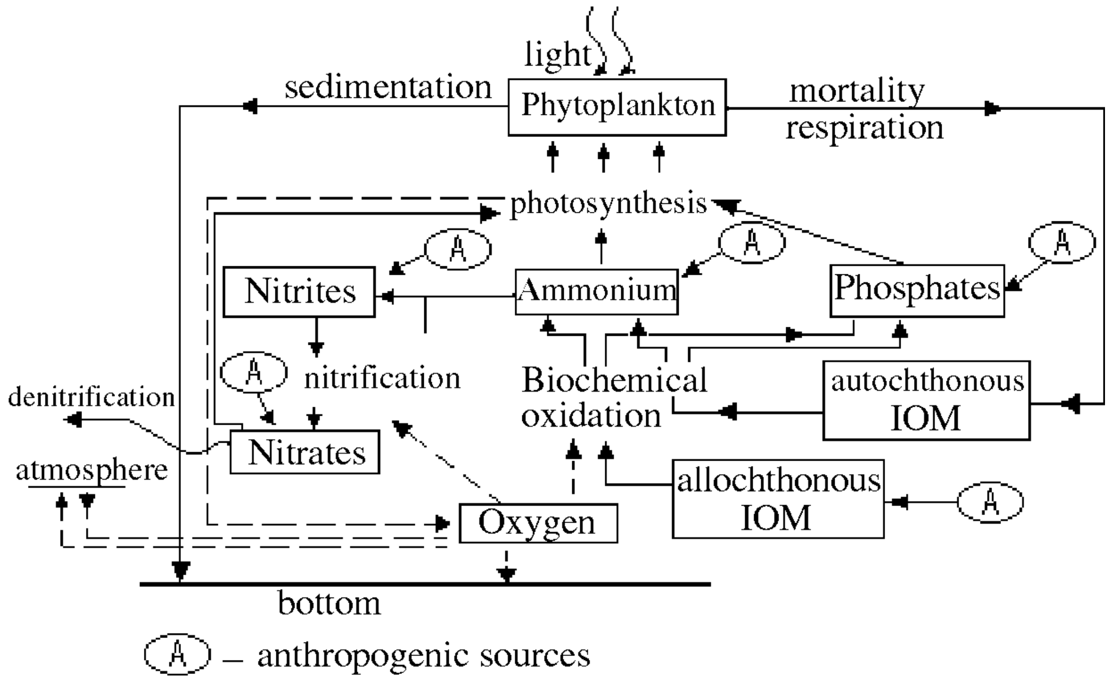


Fig. 4.1. Schematic diagram of the block of eutrophication in the model of the quality of waters of a shallow-water tropical water basin (of the Ciénaga-de-Tesca type) and the relationships between its elements (IOM stands for the inert organic matter).

The indicated assumptions are correct for the eutrophic and hypertrophic marine ecosystems in which bacterioplankton is adapted to high concentrations of the organic substrate and the trophic chain is sufficiently short. In the proposed version, the model requires minimum amounts of input data on the biotic component of the ecosystem for the description of the negative effects of the eutrophication. This is especially important for the developing countries which meet significant economic difficulties or do not have a sufficiently developed methodical base required for the realization of specialized hydrobiological observations.

In the point (zero-dimensional space) version of the block of eutrophication, the basic balance equations are written as described in what follows:

Phytoplankton B_f, $\mathrm{mgC/m^3}$. The growth of the biomass of phytoplankton occurs as a result of photosynthesis and its decrease is caused by the natural mortality of phytoplankton, its eating by zooplankton, the losses for the respiration of cells, and their gravitational sedimentation. The production of phytoplankton is limited by the illumination (transparency) of waters and the content of biogenic elements:

$$\left.\frac{dB_f}{dt}\right|_{\mathrm{loc}} = (1-\gamma_f)\sigma_f(I, C_{\mathrm{PO_4}}, C_{\mathrm{N}})B_f - \mu_f B_f - \frac{w_{gf}}{H}B_f, \tag{4.9}$$

where B_f is the biomass of phytoplankton, $\mathrm{mgC/m^3}$, t is time, h, γ_f is the fraction of production of phytoplankton spent for its vital activity (respiration), μ_f is the specific rate of natural mortality and eating of phytoplankton by the other organisms, h^{-1}, w_{gf} is the velocity of gravitational sedimentation of algae, m/h, H is depth, m, σ_f is the specific rate of growth of phytoplankton, h^{-1}, determined by the conditions of illumination I and the presence of biogenic substances (mineral compounds of nitrogen C_N and phosphorus C_{PO_4}) in water. The quantity σ_f is determined as follows:

$$\sigma_f = V_f^{max} f_i(I) f_2(C_N, C_{PO_4}), \tag{4.9a}$$

$$f_i(I) = \frac{1}{H}\int_0^H f_z(I_z)dz = \frac{2.718}{H\alpha}\left[\exp\left(-\frac{I_0}{I_{opt}}\exp(-\alpha H)\right) - \exp\left(-\frac{I_0}{I_{opt}}\right)\right], \tag{4.9b}$$

$$f_z(I_z) = \frac{I_z}{I_{opt}}\exp\left(-\frac{I_z}{I_{opt}}\right), \qquad I_z = I_0\exp(-\alpha z),$$

$$f_2(C_N, C_{PO_4}) = \min\left\{\frac{C_N}{\Pi_N + C_N}, \frac{C_{PO_4}}{\Pi_{PO_4} + C_{PO_4}}\right\}, \tag{4.9c}$$

where $C_N = C_{NH_4} + C_{NO_3}$, V_f^{max} is the maximum specific rate of growth of phytoplankton, h^{-1}, C_{PO_4}, C_{NH_4}, and C_{NO_3} are, respectively, the concentrations of phosphorus of phosphates, mgP/liter, and the ammonium and nitrate forms of nitrogen, mgN/liter, in seawater, I_0 is the flux of photosynthetically active solar radiation penetrating through the sea surface, W/m^2, I_{opt} is the irradiance optimal for the photosynthesis, W/m^2, I_z is the irradiance at depth z, W/m^2, α is the integral attenuation coefficient of the intensity of photosynthetically active radiation with depth, m^{-1}, and Π_N and Π_{PO_4} are the constants of semisaturation for the intensity of the process of utilization of the mineral compounds of nitrogen and phosphorus by phytoplankton, mgN/liter and mg/P/liter, respectively. For the ith biogenic element, the constant of semisaturation Π_i is equal to its concentration for which the rate of photosynthesis V_f is equal to a half of its maximum value, i.e.,

$$V_f = \frac{V_f^{max}}{2},$$

provided that all other conditions are optimal.

The last term on the right-side of Eq. (4.9) is included in the chemical-and-biological block only in the two-dimensional version of the model. In the three-dimensional models, the gravitational sedimentation of algae and detritus is taken into account in the block of transfer of admixtures.

Inert Organic Matter (IOM) B_{org}, $\text{mg}\,O_2/\text{liter}$, is analyzed in the model as the oxygen equivalent of the total content of organic compounds (detritus + IOM) subjected to biochemical oxidation in water. In order to take into account the difference between the ratios $C : O_2 : N : P$, the inert organic matter of natural and anthropogenic origin is studied in the model separately, i.e., $B_{\text{org}} = B_{\text{org}}^{\text{nat}} + B_{\text{org}}^{\text{ant}}$, and

$$\left.\frac{dB_{\text{org}}^{\text{nat}}}{dt}\right|_{\text{loc}} = (\gamma_f \sigma_f(I, C_{\text{PO}_4}, C_{\text{N}}) + \eta\mu_f) B_f \beta_{\text{O}_2/\text{C}} \beta_{\text{m}^3/\text{liter}} - K_{\text{BOD}}\, \varepsilon_{\text{ing}} B_{\text{org}}^{\text{nat}}, \quad (4.10\text{a})$$

$$\left.\frac{dB_{\text{org}}^{\text{ant}}}{dt}\right|_{\text{loc}} = -K_{\text{BOD}}\, \varepsilon_{\text{ing}} B_{\text{org}}^{\text{ant}} + Q_{\text{org}}^{\text{ant}} \quad (4.10\text{b})$$

where K_{BOD} is the specific rate of biochemical oxidation of the organic matter, h^{-1},

$$\varepsilon_{\text{ing}} = \frac{C_{\text{O}_2}}{C_{\text{O}_2} + \Pi_{\text{O}_2}}$$

is the parameter of deceleration of the processes of biochemical oxidation of organic matter and nitrification in the case of deficiency of oxygen in seawater $(0 < \varepsilon_{\text{ing}} < 1)$, Π_{O_2} is the constant of semisaturation of the process, $\text{mg}\,O_2/\text{liter}$, η is the fraction of labile organic substances in the dead organic matter of phytoplankton, $\beta_{O_2/\text{C}}$ is the coefficient of conversion of the carbon units of organic matter [mg C] into the oxygen units [mg O_2], $\text{mg}\,O_2/\text{mgC}$, and $Q_{\text{org}}^{\text{ant}}$ is the rate of changes in the concentration of inert organic matter caused by discharges of the anthropogenic sources, $\text{mg}\,O_2/\text{liter}\cdot\text{h}$.

Phosphorus of Phosphates C_{PO_4}, mg P/liter. Phosphorus of phosphates is consumed in the process of production of the primary organic matter by phytoplankton and regenerated in the process of biochemical oxidation of organic matter with participation of bacteria. Under aerobic conditions, phosphates can form insoluble compounds, e.g., with Fe. As a result, they are deposited in bottom sediments. Under anaerobic conditions, the process changes its direction and phosphates are released from the bottom sediments into the bulk of water. Hence,

$$\left.\frac{dC_{\text{PO}_4}}{dt}\right|_{\text{loc}} = -\sigma_f(I, C_{\text{PO}_4}, C_{\text{N}}) B_f \beta_{\text{P/C}} \beta_{\text{m}^3/\text{liter}}$$

$$+ K_{\text{BOD}}\, \varepsilon_{\text{ing}} (B_{\text{org}}^{\text{nat}} \beta_{\text{P/O}_2} + B_{\text{org}}^{\text{ant}} \beta_{\text{P/O}_2}^{\text{ant}}) + Q_{\text{PO}_4}^{\text{ant}} \pm Q_{\text{PO}_4}^{\text{sed}}, \quad (4.11)$$

where $\beta_{\text{P/C}}$ is the stoichiometric coefficient of conversion from mgC to mgP, mgP/mgC, $\beta_{\text{P/O}_2}$ and $\beta_{\text{P/O}_2}^{\text{ant}}$ are the coefficients of recalculation from mg O_2 to mg P, mgP/mgO_2, for the autochthonous organic matter B_{org}^{nat} and the organic matter of anthropogenic origin B_{org}^{ant}, respectively, $Q_{PO_4}^{ant}$ and $Q_{PO_4}^{sed}$ are the rates of changes in the concentration of phosphates, $mg\,P/liter \cdot h$, as a result of functioning of the anthropogenic sources and mass exchange with the bottom sediments, respectively, and $\beta_{m^3/liter} = 0.001$ is the coefficient of conversion from the concentrations measured in m^3 to liters.

Nitrogen of Ammonium C_{NH_4}, mgN/liter. Nitrogen of ammonium is consumed by phytoplankton in the course of primary production of organic matter and oxidized under the aerobic conditions to nitrates (first phase of nitrification). This form of mineral nitrogen is preferable for the consumption by phytoplankton. The formation of the supply of ammonium in marine media occurs as a result of both the mineralization of dead organic matter with participation of bacteria and the interaction with bottom sediments. Unlike phosphates, the penetration of ammonium from the bottom sediments occurs both under the aerobic and anaerobic conditions. Thus, we have

$$\left.\frac{dC_{NH_4}}{dt}\right|_{loc} = -\chi\sigma_f(I, C_{PO_4}, C_N)B_f\beta_{N/C}\beta_{m^3/liter} - \nu_{N_1}C_{NH_4}\varepsilon_{ing}$$

$$+ K_{BOD}\varepsilon_{ing}(B_{org}^{nat}\beta_{N/O_2} + B_{org}^{ant}\beta_{N/O_2}^{ant}) + Q_{NH_4}^{ant} + Q_{NH_4}^{sed}. \quad (4.12)$$

where ν_{N_1} is the specific rate of the first stage of nitrification, h^{-1}, $\beta_{N/C}$ is the stoichiometric coefficient of conversion from mgC to mgN, mgN/mgC, β_{N/O_2} and β_{N/O_2}^{ant} are the coefficients of recalculation from $mg\,O_2$ to mgN, $mgN/mg\,O_2$, for the autochthonous organic matter and organic matter of the anthropogenic origin, respectively, $Q_{NH_4}^{ant}$ and $Q_{NH_4}^{sed}$ are, respectively, the rates of changes in the concentration of ammonium nitrogen, $mgN/liter \cdot h$, as a result of functioning of the anthropogenic sources and mass exchange with the bottom sediments, and

$$\chi = \frac{C_{NH_4}\phi}{\phi C_{NH_4} + (1-\phi)C_{NO_3}}$$

is the fraction of mineral nitrogen consumed by phytoplankton in the form of ammonium, where, in turn, ϕ is the coefficient of preferability of the consumption of ammonium by phytoplankton relative to nitrates.

Nitrogen of Nitrites C_{NO_2}, mgN/liter. This is an intermediate form of mineral nitrogen in the process of nitrification. It is assumed that the variations of the concentration of nitrites in water are determined by the ratio of the rates of the first and second stages of nitrification. Thus, we have

$$\left.\frac{dC_{NO_2}}{dt}\right|_{loc} = \varepsilon_{ing}(\nu_{N_1}C_{NH_4} - \nu_{N_2}C_{NO_2}) + Q_{NO_2}^{ant}, \qquad (4.13)$$

where ν_{N_2} is the specific rate of the second stage of nitrification, h^{-1}, and $Q_{NO_2}^{ant}$ is the rate of changes in the concentration of nitrites caused by the discharge of the anthropogenic sources, mgN/liter·h.

Nitrogen of Nitrates C_{NO_3}, mgN/liter. Nitrogen of nitrates is the final product of the process of nitrification of mineral nitrogen and its most stable form. Under the aerobic conditions, the concentration of nitrates in the sea is determined by the intensities of their utilization by phytoplankton in the process of photosynthesis and accumulation as a result of nitrification. Under the anaerobic conditions, nitrates are reduced to molecular nitrogen as a result of the process of denitrification. According to [83], the process of photochemical reduction of nitrates can play a significant role on the sea surface. Thus, we have

$$\left.\frac{dC_{NO_3}}{dt}\right|_{loc} = \nu_{N_2}\varepsilon_{ing}C_{NO_2} - (1-\chi)\sigma_f(I, C_{PO_4}, C_N)B_f\beta_{N/C}\beta_{m^3/liter} - \upsilon_{DN}C_{NO_3} + Q_{NO_3}^{ant}, \qquad (4.14)$$

where υ_{DN} is the specific rate of decrease in the amount of nitrates, h^{-1}, as a result of the process of denitrification in waters of the bottom layer when the content of oxygen is lower than 1 mg/liter, and $Q_{NO_3}^{ant}$ is the rate of changes in the concentration of nitrates due to their supply by the anthropogenic sources, mgN/liter·h.

Dissolved Oxygen C_{O_2}, ml/liter. The dynamics of dissolved oxygen in seawater is determined by the intensity of the processes of photosynthesis, gas exchange with the atmosphere, and consumption of oxygen in the processes of nitrification and biochemical oxidation of labile organic compounds in the bulk of water and bottom sediments:

$$\left.\frac{dC_{O_2}}{dt}\right|_{loc} = \beta_{O_2/C}\sigma_f(I, C_{PO_4}, C_N)B_f\beta_{m^3/liter} - \varepsilon_{ing}(K_{BOD}B_{org} + \beta_{O_2/N_1}\nu_{N_1}C_{NH_4} + \beta_{O_2/N_2}\nu_{N_2}C_{NO_2}) - Q_{O_2}^{ant} - \frac{(Q_{O_2}^{bot} - Q_{O_2}^{atm})\beta_{m^3/liter}}{H}. \qquad (4.15)$$

where β_{O_2/N_1} and β_{O_2/N_2} are the oxygen equivalents of the first and second stages of nitrification, $mg\,O_2/mg\,N$, $Q_{O_2}^{bot}$ describes the absorption of oxygen from the unit volume of water by bottom sediments as a result of the processes of nitrification and biochemical oxidation, $mg\,O_2/m^2\cdot h$, $Q_{O_2}^{ant}$ is the decrease in the content of oxygen in the unit volume of water as a result of mixing with waste waters depleted of oxygen, $mg\,O_2/liter\cdot h$, and $Q_{O_2}^{atm}$ is the oxygen flux in the process of gas exchange with the atmosphere, $mg\,O_2/m^2\cdot h$.

In the first approximation, the absorption of oxygen by the bottom sediments can be estimated by using the empirical dependence presented in [76] on the basis of the data on the oxygen content of water C_{O_2}:

$$Q_{O_2}^{bot} = a(C_{O_2})^b, \tag{4.16}$$

where $[Q_{O_2}^{bot}] = mg/m^2\cdot h$, $[C_{O_2}] = ml/liter$, and a and b are empirical coefficients.

The oxygen exchange between the water and atmosphere is described by the formula [57]

$$Q_{O_2}^{atm} = \zeta_{e,i} n_V n_T (C_{O_2}^S - C_{O_2}), \tag{4.17}$$

where $Q_{O_2}^{atm}$ is either the penetration (invasion) or release (evasion) of oxygen, $mg/m^2\cdot h$, $\zeta_{e,i}$ is the coefficient of invasion (evasion), $liter/m^2\cdot h$, n_T is the temperature coefficient, n_V is the integral wind coefficient,

$$n_V = \begin{cases} 1.0 + 0.27W^2, & \text{for} \quad W \le 8\,m/sec, \\ -7.4 + 0.4W^2, & \text{for} \quad W > 8\,m/sec, \end{cases} \tag{4.18}$$

W is the wind velocity, m/sec, and $C_{O_2}^S$ is the saturating (for a given temperature and salinity of water) concentration of oxygen, $mg/liter$.

The outlined block of eutrophication was applied to estimate the efficiency of the alternative concepts of improvement of the ecological situation in the shallow-water tropical Ciénaga-de-Tesca Lagoon suffering powerful anthropogenic loads in the form of industrial and municipal waste waters of Cartagena (see Subsection 2.1.2) [56, 144, 159, 163]. The proposed model has a relatively simple structure and can easily be calibrated according to the experimental data and the data of *in-situ* observations (see Subsection 5.3.1). Moreover, it can be successfully used for the development of alternative concepts aimed at decreasing the level of eutrophication and improvement of the quality of waters in shallow-water basins of the marine and river types.

Since the block was developed for the tropical water basin in which the seasonal variations of the temperature of water are insignificant (do not exceed several degrees), the rates of processes are specified in the form of constants whose values for the observed temperature of water can be found in advance by using the well-known empirical dependences (see Section 5.1). However, if the model is used for the water basins of middle latitudes with well-pronounced seasonal variations of temperature, then it is necessary to introduce the rates of chemical and biological processes in the equations of the model in the form of functions of the temperature of water. This program is realized in the next subsection.

4.2.2. Block of Eutrophication for Water Areas of the Sea Located at Middle Latitudes with Separation of the Nitrogen and Phosphorus Cycles

The mathematical structure of the block described in the present subsection is based on the synthesis of the well-known theoretical [66, 80] and applied models of the quality of waters [118, 128]. In constructing the block, we take into account the fact that the rates of the processes of phosphatization and ammonification of organic matter can be different. In order to separate the nitrogen and phosphorus cycles, we introduce in the model two additional sufficiently informative characteristics, namely, the concentrations of the organic compounds of phosphorus and nitrogen. The measurements of these concentrations are included in the complex of ecological monitoring. The inclusion of these variables in the structure of the model allows us to automatically take into account possible differences between the ratios of the contents of nitrogen and phosphorus in the composition of autochthonous and allochthonous organic matter (including the substances coming from the anthropogenic sources). The combination of nitrogen and phosphorus cycles in a single model is realized on the basis of the equation of dynamics of phytoplankton used to describe the primary production of organic matter by phytoplankton in the process of photosynthesis and the replenishment of the amounts of inert organic matter (in the nitrogen and phosphorus units) as a result of the processes of respiration, natural mortality, and eating of phytoplankton by the other organisms.

Note that the specific rates of chemical and biological processes are regarded as functions of the parameters of state of the marine medium but not as constants. The inert organic matter (represented in the nitrogen, phosphorus, and oxygen units) is separated into the detrital and dissolved parts. The detrital part of the inert organic matter undergoes gravitational sedimentation.

Since the analyzed block is developed as a part of the three-dimensional model of the quality of waters in the sea, the equations of the biotic component of the ecosystem are closed on the level of phytoplankton in order to preserve the computational properties of the model. However, the model enables us to describe the dynamics not of a single group of phytoplankton but of its several systematic groups typical of the ecosystem, i.e., of its successions.

In the version proposed for the Dnieper–Bug estuary region in the northwest part of the Black Sea, the model of eutrophication includes 11 chemical and biological elements: phytoplankton B_f, phosphates C_{PO_4}, nitrogen of ammonium C_{NH_4}, nitrogen of nitrates C_{NO_3}, dissolved organic phosphorus C_{DOP}, dissolved organic nitrogen C_{DON}, particulate organic phosphorus C_{POP}, particulate organic nitrogen C_{PON}, detrital $B_{\mathrm{org}}^{\mathrm{det}}$ and dissolved $B_{\mathrm{org}}^{\mathrm{dis}}$ forms of the oxygen equivalent of inert organic matter [biochemical oxygen demand (BOD), permanganate oxidizability], and dissolved oxygen $C_{\mathrm{O_2}}$. The nitrogen of nitrites is combined with the nitrogen of nitrates. We also compute the parameter $\mathrm{BOD_5}$. The block diagram of relationships between the elements of the model is presented in Fig. 4.2.

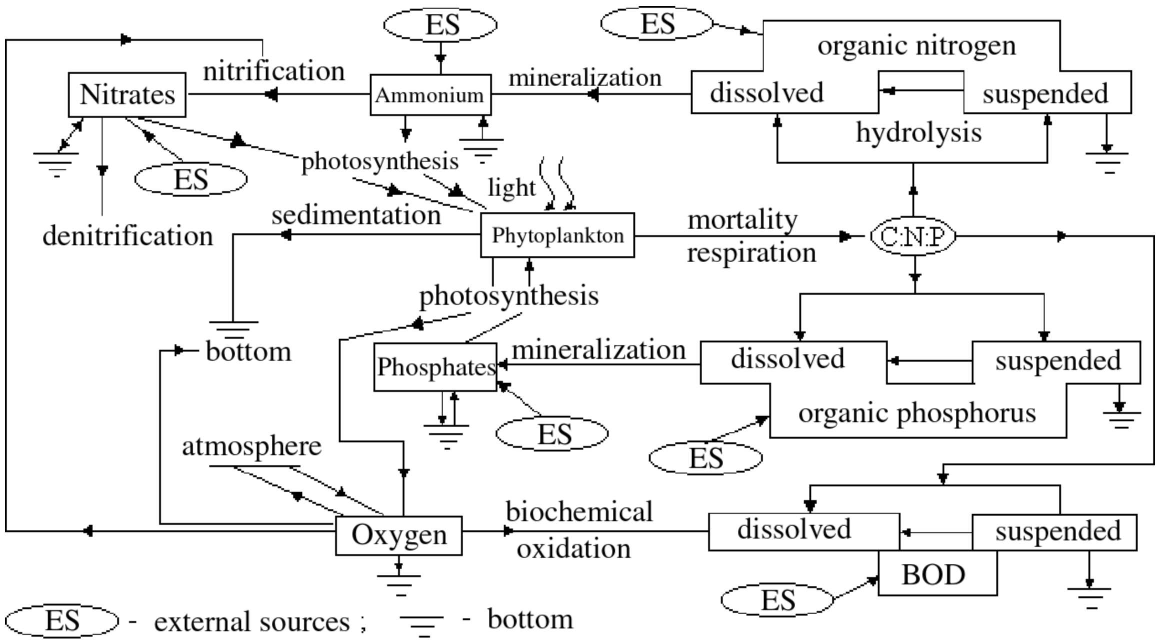


Fig. 4.2. Block diagram of relationships between the elements of the block of eutrophication of the model of the quality of waters for the northwest part of the Black Sea.

The system of equations of the block of eutrophication for a local point of the space is described in what follows.

Phytoplankton, $\mathrm{gC/m^3}$:

$$\left.\frac{dB_f}{dt}\right|_{\mathrm{loc}} = (\sigma_f - \varphi_f - \mu_f)B_f, \tag{4.19}$$

where $\sigma_f = V_f^{\max} f_1(I) f_2(C_{\mathrm{N}}, C_{\mathrm{PO_4}}) f_3(T)$,

$$f_1(I) = \frac{1}{\Delta z}\int_{z_i}^{z_{i+1}} f_z(I_z)dz = \frac{2.718 f_d}{\Delta z \alpha}[\exp(-R_{z_i}) - \exp(-R_{z_{i+1}})], \tag{4.19a}$$

$$R_0 = \frac{I_a}{I_{\text{opt}}}, \quad R_{z_i} = R_0 \exp(-\alpha z_i), \quad \Delta z = z_{i+1} - z_i,$$

$$f_z(I_z) = \frac{I_z}{I_{\text{opt}}} \exp\left(1 - \frac{I_z}{I_{\text{opt}}}\right), \quad I_z = I_a \exp(-\alpha z),$$

$$f_2(C_{\text{N}}, C_{\text{PO}_4}) = \min\left\{\frac{C_{\text{N}}}{\Pi_{\text{N}} + C_{\text{N}}}, \frac{C_{\text{PO}_4}}{\Pi_{\text{PO}_4} + C_{\text{PO}_4}}\right\}, \tag{4.19b}$$

where $C_{\text{N}} = C_{\text{NH}_4} + C_{\text{NO}_3}$,

$$f_3(T) = \begin{cases} e^{-\varsigma_1 (T - T_m)^2} & \text{for} \quad T \le T_m, \\ e^{-\varsigma_2 (T_m - T)^2} & \text{for} \quad T > T_m, \end{cases} \tag{4.19c}$$

$$\varphi_f = \varphi_r e^{\varsigma_\varphi (T - T_r)}, \tag{4.20}$$

$$\mu_f = \mu_r e^{\varsigma_\mu (T - T_r)}, \tag{4.21}$$

Here, I_a is the daily average flux of photosynthetically active radiation penetrating through the sea surface, W/m^2, f_d is the fraction of daytime in 24 h $(0 \le f_d \le 1)$, φ_f is the specific rate of metabolism (respiration), day^{-1}, T is the temperature of seawater, °C, T_m is the temperature of seawater optimal for the growth of algae, °C, ς_1 and ς_2 are coefficients specifying the character of influence of temperature on the growth of algae at temperatures higher and lower than T_m, $1/(°\text{C})^2$, φ_r is the specific rate of metabolism of algae at a temperature T_r, day^{-1}, ς_φ is the coefficient of influence of temperature on the rate of metabolism, $(°\text{C})^{-1}$, μ_r is the specific rate of eating and death of phytoplankton at the temperature T_r, day^{-1}, and ς_μ is the coefficient of influence of temperature on the rate of eating and death of algae, $(°\text{C})^{-1}$.

The remaining notation used in what follows correspond to the notation introduced in Subsection 4.2.1.

Phosphorus of Phosphates, gP/m^3. We have

$$\left.\frac{dC_{\text{PO}_4}}{dt}\right|_{\text{loc}} = (\varphi_f \alpha_p + \mu_f g_{p1} - \sigma_f)\beta_{\text{P/C}} B_f + K_{\text{PO}_4} C_{\text{DOP}}, \tag{4.22}$$

where α_p is the fraction of phosphates in the metabolic excretions of algae $(0 \le \alpha_p \le 1)$, g_{p1} is the fraction of phosphates produced as a result of eating and mortality of phytoplankton $(0 \le g_{p1} \le 1)$, $\beta_{P/C}$ is the coefficient used to express the stoichiometric ratio of carbon and phosphorus in the organic matter, gP/gC, K_{PO_4} is the specific rate of mineralization of dissolved organic phosphorus, day^{-1}, given by the formula

$$K_{PO_4} = K_{PO_4}^{20}\left(\frac{B_f}{\Pi_C + B_f}\right)\theta_{PC}^{(T-20)},$$

where $K_{PO_4}^{20}$ is the specific rate of mineralization of dissolved organic phosphorus at 20°C, day^{-1}, θ_{PC} is a temperature coefficient, and Π_C is the constant of semisaturation specifying the limiting influence of the biomass of phytoplankton on the regeneration of mineral compounds of phosphorus and nitrogen [128], gC/m^3.

Nitrogen of Ammonium, gN/m^3. We have

$$\left.\frac{dC_{NH_4}}{dt}\right|_{loc} = (\varphi_f\alpha_N + \mu_f g_{N1} - \chi\sigma_f)\beta_{N/C}B_f + K_{NH_4}C_{DON} - \nu_{12}C_{NH_4}, \quad (4.23)$$

where α_N is the fraction of nitrogen of ammonium in the metabolic excretions of algae, g_{N1} is the fraction of nitrogen of ammonium produced as a result of eating and mortality of phytoplankton, χ is the fraction of mineral nitrogen consumed by phytoplankton in the form of ammonium given by the formula

$$\chi = C_{NH_4}\frac{C_{NO_3}}{(\Pi_N + C_{NH_4})(\Pi_N + C_{NO_3})} + C_{NH_4}\frac{\Pi_N}{(C_{NH_4} + C_{NO_3})(\Pi_N + C_{NO_3})},$$

$\beta_{N/C}$, gN/gC, is the stoichiometric ratio of carbon and nitrogen in the organic matter, K_{NH_4}, day^{-1}, is the specific rate of mineralization of organic nitrogen given by the formula

$$K_{NH_4} = K_{NH_4}^{20}\left(\frac{B_f}{\Pi_C + B_f}\right)\theta_{NC}^{(T-20)},$$

$K_{NH_4}^{20}$, day^{-1}, is the specific rate of mineralization of organic nitrogen for a water temperature of 20°C, θ_{NC} is a temperature coefficient, ν_{12}, day^{-1}, is the specific rate of nitrification given by the formula

$$\nu_{12} = \nu_{12}^{20}\varepsilon_{ing}\theta_{NIT}^{(T-20)},$$

ν_{12}^{20}, day^{-1}, is the specific rate of nitrification at a temperature of 20°C, θ_{NIT} is a temperature coefficient,

$$\varepsilon_{\text{ing}} = \frac{C_{\text{O}_2}}{\Pi_{\text{O}_2} + C_{\text{O}_2}}$$

is a factor taking into account the limiting influence of the amount of oxygen dissolved in water on the process of nitrification, and Π_{O_2} is the constant of semisaturation of the process relative to the available concentration of oxygen, $\text{g}\,\text{O}_2/\text{m}^3$.

Nitrogen of Nitrates, gN/m^3. We have

$$\left.\frac{dC_{\text{NO}_3}}{dt}\right|_{\text{loc}} = (\chi - 1)\sigma_f \beta_{\text{N/C}} B_f + \nu_{12} C_{\text{NH}_4} - \upsilon_{DN} C_{\text{NO}_3}, \qquad (4.24)$$

where υ_{DN}, day^{-1}, is the specific rate of the process of denitrification given by the formula

$$\upsilon_{DN} = \upsilon_{DN}^{20} \frac{\Pi_{DN}}{\Pi_{DN} + C_{\text{O}_2}} \theta_{DN}^{(T-20)},$$

υ_{DN}^{20}, day^{-1}, is the specific rate of denitrification at a temperature of 20°C, θ_{DN} is a temperature coefficient, Π_{DN}, $\text{g}\,\text{O}_2/\text{m}^3$, is a constant taking into account the influence of the amount of oxygen dissolved in water on the rate of the process of denitrification.

Dissolved Organic Phosphorus, gP/m^3. We have

$$\left.\frac{dC_{\text{DOP}}}{dt}\right|_{\text{loc}} = (\varphi_f (1 - \alpha_P) + \mu_f g_{P2}) \beta_{\text{P/C}} B_f + \delta_P C_{\text{POP}} - K_{\text{PO}_4} C_{\text{DOP}}. \qquad (4.25)$$

where g_{P2} is the fraction of dissolved organic phosphorus supplied as a result of mortality of phytoplankton and its eating by the other organisms, g_P is the specific rate of hydrolysis of labile particulate organic phosphorus regarded as a function of the temperature of water, $g_P = g_P^{20} \theta_{\text{par}}^{(T-20)}$, where g_P^{20} is the rate of hydrolysis at a temperature of 20°C, and θ_{par} is a temperature coefficient.

Labile Particulate Organic Phosphorus, gP/m^3. We have

$$\left.\frac{dC_{\text{POP}}}{dt}\right|_{\text{loc}} = \mu_f g_{P3} \beta_{\text{P/C}} B_f - \delta_P C_{\text{POP}}, \qquad (4.26)$$

where g_{P3} is the fraction of labile particulate phosphorus produced as a result of eating of phytoplankton and its mortality. Note that $g_{P1} + g_{P2} + g_{P3} < 1$ because the model studies solely the labile part of the inert organic matter.

Dissolved Organic Nitrogen, gN/m^3. We have

$$\left.\frac{dC_{\mathrm{DON}}}{dt}\right|_{\mathrm{loc}} = (\varphi_f(1-\alpha_N) + \mu_f g_{N2})\beta_{\mathrm{N/C}} B_f + \delta_N C_{\mathrm{PON}} - K_{\mathrm{NH}_4} C_{\mathrm{DON}}, \quad (4.27)$$

where g_{N2} is the fraction of dissolved organic nitrogen supplied as a result of eating and mortality of phytoplankton and δ_N, day^{-1}, is the specific rate of hydrolysis of labile particulate organic nitrogen determined by analogy with the phosphorus cycle.

Labile Particulate Organic Nitrogen, gN/m^3. We have

$$\left.\frac{dC_{\mathrm{PON}}}{dt}\right|_{\mathrm{loc}} = \mu_f g_{N3}\beta_{\mathrm{N/C}} B_f - \delta_N C_{\mathrm{PON}}, \quad (4.28)$$

where g_{N3} is the fraction of labile particulate nitrogen produced as a result of eating and mortality of phytoplankton.

Dissolved Part of the Biochemical Oxygen Demand (BOD), gO_2/m^3. In the model, this parameter is regarded as the oxygen equivalent of dissolved organic carbon. We have

$$\left.\frac{dB_{\mathrm{org}}^{\mathrm{dis}}}{dt}\right|_{\mathrm{loc}} = (\alpha_C\varphi_f + \mu_f g_{C2})\beta_{\mathrm{O_2/C}} B_f + \delta_C B_{\mathrm{org}}^{\mathrm{det}} - K_{\mathrm{BOD}} B_{\mathrm{org}}^{\mathrm{dis}} - \beta_{\mathrm{O_2}/DN} \upsilon_{DN} C_{\mathrm{NO_3}}, \quad (4.29)$$

where α_C is the fraction of dissolved organic matter in the metabolic excretions of algae, g_{C2} is the fraction of dissolved organic carbon supplied as a result of eating and mortality of phytoplankton, $\delta_C = \delta_C^{20}\theta_C^{(T-20)}$ is the specific rate of dissolution of labile particulate organic carbon, day^{-1}, δ_C^{20} is the specific rate of dissolution at a temperature of 20°C, θ_C is a temperature coefficient of the process, K_{BOD}, day^{-1}, is the specific rate of biochemical oxidation of organic matter given by the formula $K_{\mathrm{BOD}} = K_{\mathrm{BOD}}^{20}\theta_{\mathrm{BOD}}^{(T-20)}\varepsilon_{\mathrm{ing}}$, K_{BOD}^{20}, day^{-1}, is the specific rate of biochemical oxidation for $T = 20$°C, θ_{BOD} is a temperature coefficient, and $\beta_{\mathrm{O_2}/DN}$, gO_2/gN, is the oxygen equivalent of organic carbon in the reaction of denitrification.

Detrital Part of BOD, gO_2/m^3. We have

$$\left.\frac{dB_{\mathrm{org}}^{\mathrm{det}}}{dt}\right|_{\mathrm{loc}} = \mu_f g_{C3}\beta_{\mathrm{O_2/C}} B_f - \delta_C B_{\mathrm{org}}^{\mathrm{det}}, \quad (4.30)$$

where g_{C3} is the fraction of labile particulate organic carbon supplied as a result of eating and mortality of phytoplankton.

Dissolved Oxygen, gO_2/m^3. We have

$$\left.\frac{dC_{O_2}}{dt}\right|_{loc} = [\sigma_f(1.3 - 0.3\chi) - (1 - \alpha_C)\varphi_f)\beta_{O_2/C}B_f - K_{BOD}B_{org}^{dis} - \nu_{12}C_{NH_4}\beta_{O_2/NT}, \quad (4.31)$$

where $\beta_{O_2/NT}$, gO_2 /gN, is the oxygen equivalent of the process of nitrification.

BOD₅, gO_2/m^3. This quantity is, in fact, formal. It is included in the model as one of the most extensively used hydrochemical parameters of the quality of waters. For its evaluation, we use the following diagnostic formula:

$$\mathrm{BOD}_5 = B_{org}^{dis}(1 - e^{-5K_{BOD}^{lab}}) + \beta_{O_2/NT}C_{NH_4}(1 - e^{-5\nu_{12}^{lab}}) + \beta_{O_2/C}B_f(1 - e^{-5\varphi_f^{lab}}), \quad (4.32)$$

where K_{BOD}^{lab}, ν_{12}^{lab}, and φ_f^{lab} are the specific rates of the processes of biochemical oxidation of organic matter, nitrification, and respiration of phytoplankton under the laboratory conditions of incubation of samples.

The block of eutrophication also enables us to find the fluxes of oxygen on the upper and lower boundaries of the water column and study the mass exchange by biogenic elements between the bottom sediments and water.

The oxygen exchange with the atmosphere is analyzed by using relation (4.17). The absorption of oxygen by the bottom sediments is described by the formula [128]

$$Q_{O_2}^{bot} = \frac{C_{O_2}^b}{\Pi_{O_2} + C_{O_2}^b} Q_{O_2}^{Tb} e^{\varsigma_o(T - T_b)}, \quad (4.33)$$

where $Q_{O_2}^{Tb}$, $gO_2/m^2\cdot day$, is the flux of absorption of oxygen by the bottom sediments for the temperature of the bottom water T_b, °C, $C_{O_2}^b$, gO_2/m^3, is the oxygen content of the bottom layer, ς_o is the coefficient of influence of temperature on the absorption of oxygen by the bottom sediments, $(°C)^{-1}$.

The flux of nitrates in the "water–bottom-sediments" system is determined by the ratio of their concentrations in water and bottom sediments, the rate of the process of mass exchange through the boundary, and the intensity of the process of denitrification in bottom sediments [128]:

$$Q_{NO_3}^{bot} = k_{sw}(C_{NO_3}^{bot} - C_{NO_3}^b)e^{\varsigma_{dn}(T - T_{rNO_3})}, \quad (4.34)$$

where k_{sw}, m/day, is the rate of mass transfer through the "water–bottom-sediments" boundary, $C^{b}_{NO_3}$, gN/m^3, is the concentration of nitrates in the porous water of bottom sediments $C^{bot}_{NO_3}$, gN/m^3, is the concentration of nitrates in bottom waters, ς_{dn}, $(°C)^{-1}$, is the coefficient of influence of temperature on the rate of denitrification, and T_{rNO_3} is the temperature of measuring the flux of nitrates.

The model takes into account the influence of temperature on the fluxes of ammonium nitrogen and phosphates in the "water–bottom sediments" system specified by the user:

$$Q^{bot}_{C_i} = Q^{br}_{C_i} e^{\varsigma_{C_i}(T - T_{br})}. \tag{4.35}$$

where $Q^{bot}_{C_i}$, $g/m^2 \cdot day$, is the bottom flux of a substance C_i at temperature T, $Q^{b}_{C_i}$, $g/m^2 \cdot day$, is the bottom flux of the substance C_i at temperature T_{br}, and ς_{C_i}, $(°C)^{-1}$, is a temperature coefficient.

The dependence of the intensity of mass exchange with bottom sediments on the temperature of water is explained by the fact that, at middle latitudes, the rates of mineralization of the organic matter accumulated in the bottom sediments increase in the process of heating of the bottom waters in the spring–summer period and this leads to the intensification of the fluxes of mineral compounds of biogenic elements from the bottom sediments into the bulk of water and the flux of absorption of oxygen by the bottom sediments.

4.2.3. Block of Eutrophication for the Tropical Shelf Marine Ecosystems with Regard for Bacterioplankton

In the present subsection, we consider the block of eutrophication in which bacterioplankton is regarded as a component of the model. Parallel with phytoplankton, bacterioplankton plays an extremely important role in the process of functioning of water ecosystems. Thus, on the one hand, bacteria utilize the inert autochthonous and allochthonous organic matter as a source of substance and energy. On the other hand, the mineral compounds of nitrogen and phosphorus are regenerated as a result of the metabolic activity of bacteria. Moreover, the amount of inert organic matter biochemically oxidized by bacteria to satisfy their energy demand is three times greater than the amount required for the construction of their cells. The production of bacteria is determined by the availability of inert organic matter, temperature, and oxygen conditions. The biomass of bacteria decreases as a result of their eating by zooplankton and natural mortality.

The inclusion of bacteria in the model and explicit description of their role in the mineralization of organic matter enables us to take into account the effect of inhomogeneity of the space distribution of the biomass of bacteria on the concentration of organic matter, the rate of its biochemical oxidation, the rate of regeneration of the mineral compounds of biogenic elements, and the rate of consumption of oxygen. In this aspect, the proposed structure of the biochemical block of the model is, to a significant extent, more complex and systematic than the structure of the models of eutrophication traditionally used in the engineering practice in which the rate of oxidation of the inert organic matter is regarded as a constant independent of the functional characteristics of bacteria and their available biomass.

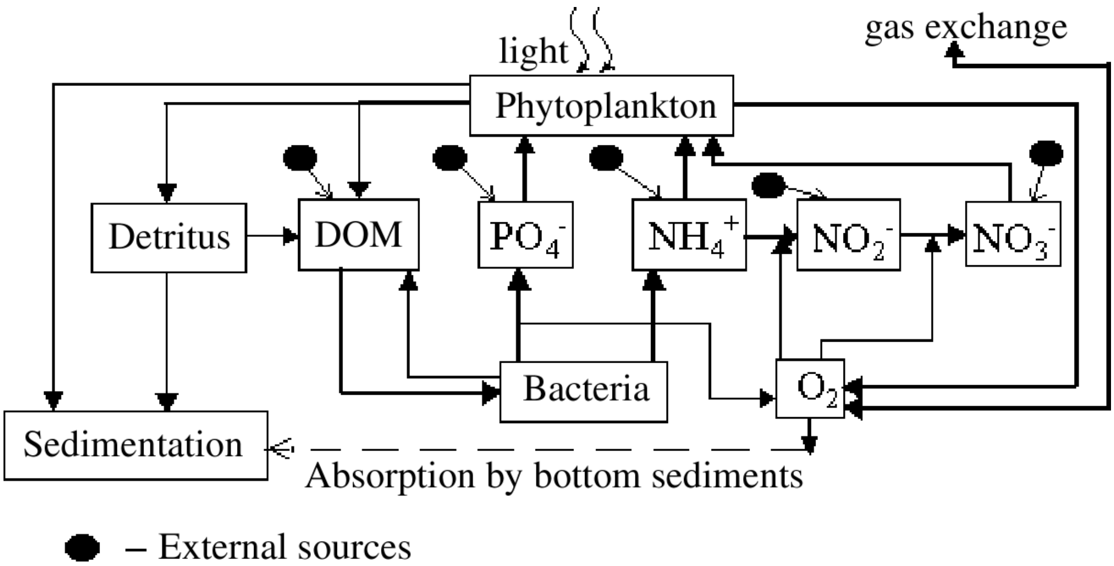


Fig. 4.3. Schematic diagram of the block of eutrophication in the model of the quality of waters in the Cartagena Bay.

The block of eutrophication of the three-dimensional model of the quality of waters developed for the deep-water marine Cartagena Bay includes the following components of the ecosystem: phytoplankton B_f, bacterioplankton B_b, detritus $B_{\text{org}}^{\text{det}}$, $B_{\text{org}}^{\text{dis}} = B_{\text{org}}^{\text{ant}} + B_{\text{org}}^{\text{nat}}$, where $B_{\text{org}}^{\text{nat}}$ is the dissolved organic matter (DOM) of the natural origin and $B_{\text{org}}^{\text{ant}}$ is the DOM of the anthropogenic origin, phosphates C_{PO_4}, ammonium C_{NH_4}, nitrites C_{NO_2}, nitrates C_{NO_3}, and dissolved oxygen C_{O_2}. The diagram of relationships between the components of the ecosystem is presented in Fig. 4.3.

Since the Cartagena Bay is a tropical marine water basin of tidal type, the time step used in the block of eutrophication is set equal to 1 h, and the temperature dependences of the parameters of the model are taken into account in the stage of precalibration of the model.

The equations of the block for a local point of the space are presented in what follows.

Phytoplankton, mgC/m^3. We have

$$\left.\frac{dB_f}{dt}\right|_{\text{loc}} = (1-\gamma_f)\sigma_f(I, C_{\text{PO}_4}, C_{\text{N}})B_f - \mu_f B_f, \tag{4.36}$$

where

$$\sigma_f = V_f^{\max} f_1(I) f_2(C_{\rm N}, C_{\rm PO_4})$$

and the factors f_1 and f_2 are determined by relations (4.19a) and (4.19b). The remaining parameters of the equations and notation not mentioned here and in what follows are similar to the corresponding quantities introduced in Subsection 4.2.

Bacterioplankton, $\mathrm{mgC/m^3}$. We have

$$\left.\frac{dB_b}{dt}\right|_{\rm loc} = V_b^{\max}\left(\frac{B_{\rm org}^{\rm dis}}{\Pi_{\rm org} + B_{\rm org}^{\rm dis}} - \frac{B_b}{B_b^{\max}}\right)B_b, \tag{4.37}$$

where B_b and $B_b^{\max}$ are the current and maximally possible biomass of bacteria, $V_b^{\max}$, $\mathrm{h^{-1}}$, is the maximum specific rate of growth of bacterioplankton,

$$\mu_b = V_b^{\max}\frac{B_b}{B_b^{\max}}$$

is the specific rate of natural mortality of bacterioplankton, $\mathrm{h^{-1}}$, $\Pi_{\rm org}$, $\mathrm{mg\,O_2/liter}$, is the constant of semisaturation of the growth of bacteria equal to the concentration of the organic substrate for which the actual specific growth rate of bacteria is equal to a half of its maximum value, $B_{\rm org}^{\rm dis}$, $\mathrm{mgO_2/liter}$, is the concentration of DOM (formed by the organic substances of the anthropogenic $B_{\rm org}^{\rm ant}$ and natural $B_{\rm org}^{\rm nat}$ origin) in seawater.

The structure of Eq. (4.37) takes into account the influence of density of the population of bacteria on their mortality. For the values of B_b small as compared with $B_b^{\max}$, Eq. (4.37) turns into the well-known Monod equation. At the same time, for the values of $B_{\rm org}^{\rm dis}$ greater than $\Pi_{\rm org}$, Eq. (4.37) transforms into the equation of logistic growth and, hence, acquires the required flexibility [67].

Inert Organic Matter (IOM), $\mathrm{mg\,O_2/liter}$. We have

$$\left.\frac{dB_{\rm org}^{\rm det}}{dt}\right|_{\rm loc} = \lambda_f \eta_f \mu_f B_f \beta_{\rm O_2/C}\beta_{\rm m^3/liter} - \delta B_{\rm org}^{\rm det}, \tag{4.38}$$

$$\left.\frac{dB_{\rm org}^{\rm nat}}{dt}\right|_{\rm loc} = \Big[(\gamma_f \sigma_f(I, C_{\rm PO_4}, C_{\rm N}) + (1-\lambda_f)\eta_f\mu_f)B_f + \mu_b B_b$$

$$- \frac{V_b^{\max}}{E}\frac{B_{\rm org}^{\rm nat}}{\Pi_{\rm org} + B_{\rm org}^{\rm dis}} B_b \varepsilon_{\rm ing}\Big]\beta_{\rm O_2/C}\beta_{\rm m^3/liter} + \delta B_{\rm org}^{\rm det}, \tag{4.39}$$

$$\left.\frac{dB_{\text{org}}^{\text{ant}}}{dt}\right|_{\text{loc}} = Q_{\text{org}}^{\text{ant}} - \frac{V_b^{\max}}{E}\frac{B_{\text{org}}^{\text{ant}}}{Bk_{\text{org}} + B_{\text{org}}^{\text{dis}}} B_b \varepsilon_{\text{ing}} \beta_{\text{O}_2/\text{C}} \beta_{\text{m}^3/\text{liter}}, \tag{4.40}$$

where $B_{\text{org}}^{\text{det}}$, $\text{mgO}_2/\text{liter}$, is the concentration of particulate IOM (detritus), δ, h^{-1}, is the specific rate of autolysis of detritus, λ_f is the fraction of the detritus in the remains of dead cells of phytoplankton $(0 < \lambda_f < 1)$,

$$\mu_b = V_b^{\max} \frac{B_b^2}{B_b^{\max}},$$

is the specific rate of mortality of bacterioplankton, h^{-1}, E is a dimensionless (economic) coefficient specifying the fraction of consumed energy spent for the growth of bacteria and given by the formula

$$E = \frac{P_b}{P_b + R_b},$$

where $P_b + R_b$ is the energy consumed by bacteria and P_b and R_b are its fractions spent for the production and metabolism, respectively [67].

Phosphorus of Phosphates, mgP/liter. We have

$$\left.\frac{dC_{\text{PO}_4}}{dt}\right|_{\text{loc}} = \left[\left(\frac{1}{E} - 1\right)\beta_{\text{P/C}} B_{\text{org}}^{\text{nat}} + \left(\frac{1}{E} - \omega_P\right)\beta_{\text{P/C}}^{\text{ant}} B_{\text{org}}^{\text{ant}}\right] \frac{V_b^{\max}}{\Pi_{\text{org}} + B_{\text{org}}^{\text{dis}}} B_b \beta_{\text{m}^3/\text{liter}} \varepsilon_{\text{ing}}$$

$$- \sigma_f(I, C_{\text{PO}_4}, C_{\text{N}}) B_f \beta_{\text{P/C}} \beta_{\text{m}^3/\text{liter}} + Q_{\text{PO}_4}^{\text{ant}}. \tag{4.41}$$

Nitrogen of Ammonium, mgN/liter. We have

$$\left.\frac{dC_{\text{NH}_4}}{dt}\right|_{\text{loc}} = \left[\left(\frac{1}{E} - 1\right) B_{\text{org}}^{\text{nat}} \beta_{\text{N/C}}\right.$$

$$\left. + \left(\frac{1}{E} - \omega_N\right) B_{\text{org}}^{\text{ant}} \beta_{\text{N/C}}^{\text{ant}}\right] \frac{V_b^{\max}}{\Pi_{\text{org}} + B_{\text{org}}^{\text{dis}}} B_b \beta_{\text{m}^3/\text{liter}} \varepsilon_{\text{ing}}$$

$$- \chi\sigma_f(I, C_{\text{PO}_4}, C_{\text{N}}) B_f \beta_{\text{N/C}} \beta_{\text{m}^3/\text{liter}} - \nu_{N1} C_{\text{NH}_4} \varepsilon_{\text{ing}} + Q_{\text{NH}_4}^{\text{ant}}, \tag{4.42}$$

where

$$\omega_P = \frac{\beta_{\mathrm{P/C}}}{\beta_{\mathrm{P/C}}^{\mathrm{ant}}} \quad \text{and} \quad \omega_{\mathrm{N}} = \frac{\beta_{\mathrm{N/C}}}{\beta_{\mathrm{N/C}}^{\mathrm{ant}}}$$

are the ratios of the concentrations of phosphorus and nitrogen of natural and anthropogenic origin in the organic matter, respectively, and $\beta_{\mathrm{P/C}}$, $\beta_{\mathrm{N/C}}$, $\beta_{\mathrm{P/C}}^{\mathrm{ant}}$, and $\beta_{\mathrm{N/C}}^{\mathrm{ant}}$ are, respectively, the stoichiometric coefficients of conversion from mgC into mgP and mgN for the inert organic matter of natural ($B_{\mathrm{org}}^{\mathrm{nat}}$) and anthropogenic ($B_{\mathrm{org}}^{\mathrm{ant}}$) origin in mgP/mgC and mgN/mgC.

The first term on the right-hand side of Eqs. (4.41) and (4.42) describes the regeneration of the mineral compounds of phosphorus and nitrogen in the process of metabolism of bacteria because

$$R_b = \left(\frac{1}{E} - 1\right) P_b,$$

where R_b are the losses for metabolism (respiration) and P_b is the production of bacteria. In this case, we take into account the fact that the bacteria oxidize several times more organic matter than it is necessary for the construction of their cells [65, 67].

Nitrogen of Nitrites, mgN/liter. We have

$$\left.\frac{dC_{\mathrm{NO}_2}}{dt}\right|_{\mathrm{loc}} = \nu_{N1} C_{\mathrm{NH}_4} \varepsilon_{\mathrm{ing}} - \nu_{N2} C_{\mathrm{NO}_2} \varepsilon_{\mathrm{ing}} + Q_{\mathrm{NO}_2}^{\mathrm{ant}}. \tag{4.43}$$

Nitrogen of Nitrates, mgN/liter. We have

$$\left.\frac{dC_{\mathrm{NO}_3}}{dt}\right|_{\mathrm{loc}} = \nu_{N2} C_{\mathrm{NO}_2} \varepsilon_{\mathrm{ing}} - (1-\chi)\sigma_f(I, C_{\mathrm{PO}_4}, C_{\mathrm{N}}) B_f \beta_{\mathrm{N/C}} \beta_{\mathrm{m}^3/\mathrm{liter}}$$

$$- \upsilon_{DN}(C_{\mathrm{NO}_3} - C_{\mathrm{NO}_3}^{\mathrm{crit}}) - \upsilon_{\mathrm{phot}}(C_{\mathrm{NO}_3} - C_{\mathrm{NO}_3}^{\mathrm{crit}}) + Q_{\mathrm{NO}_3}^{\mathrm{ant}}. \tag{4.44}$$

where υ_{phot}, h^{-1}, is the specific rate of decrease in the concentration of nitrates as a result of the physicochemical processes running in the surface layer and $C_{\mathrm{NO}_3}^{\mathrm{crit}}$, mgN/liter, is the minimum concentration of nitrates for which the processes of their reduction are terminated.

Dissolved Oxygen, mg O_2/liter. We have

$$\left.\frac{dC_{\mathrm{O}_2}}{dt}\right|_{\mathrm{loc}} = \left[\sigma_f(I, C_{\mathrm{PO}_4}, C_{\mathrm{N}}) B_f - \frac{V_b^{\max}}{E} \frac{B_{\mathrm{org}}^{\mathrm{dis}}}{\Pi_{\mathrm{org}} + B_{\mathrm{org}}^{\mathrm{dis}}} B_b \varepsilon_{\mathrm{ing}}\right] \beta_{\mathrm{O}_2/\mathrm{C}} \beta_{\mathrm{m}^3/\mathrm{liter}}$$

$$- (\beta_{O_2/N1} \nu_{N1} C_{NH_4} + \nu_{N2} \beta_{O_2/N2} C_{NO_2}) \varepsilon_{ing} - (Q_{O_2}^{bot} - Q_{O_2}^{atm}) \beta_{m^3/liter}. \quad (4.45)$$

The oxygen exchange with the atmosphere is described by relation (4.17). The absorption of oxygen by the bottom sediments is described by relation (4.16) modified as follows:

$$Q_{O_2}^{bot} = a f(x, y)(C_{O_2})^b, \quad (4.46)$$

where $[Q_{O_2}^{bot}] = mg/m^2 \cdot h$, $[C_{O_2}] = ml/liter$, $a = const$ and $b = const$ are empirical coefficients, and $f(x)$ is a function used to describe the space variations of the flux of absorption of oxygen by the bottom sediments and defined as follows:

$$f(x, y) = \frac{F_{org}^{act}(x, y)}{F_{med}^{act}},$$

where $F_{org}^{act}(x, y)$ is the flux of organic matter into the bottom sediments computed according to the model at each point of observations in the case of stationary external loads acting upon the ecosystem and stable hydrometeorological conditions, and $F_{med}^{act}(x, y)$ is the mean value of the flux of organic matter under current conditions determined either as a result of special experiments or in the process of calibration of the model.

The modified equation (4.46) enables us to determine the amount of oxygen absorbed by the bottom sediments more precisely on the basis of the data on the flux of organic matter into the bottom sediments determined in the model for every point of the analyzed region.

4.2.4. Complex Block of Eutrophication for Tropical Marine Basins with Regard for Bacterioplankton and Zooplankton

The model in which the equations of the block of eutrophication are closed on the level of phytoplankton regarded as the principal biotic element specifying the variability of the state of waters in ecosystems does not allow one to adequately reproduce in the model the annual dynamics of the chemical and biological parameters of the quality of waters in the ecosystems with stressed trophic links between phyto- and zooplankton. As symptoms of this situation, we can mention an approximate equality of the typical biomasses of phyto- and zooplankton or even higher values of the biomass of zooplankton (as indicated, e.g., in [44]). In this case, zooplankton not only affects the dynamics of the variables of state of an ecosystem but also plays the role of a large pool of organic matter that should be taken into account in the structure of the model as an important element of the marine ecosystem.

Most often, the biomass of zooplankton should be taken into account in the process of modeling of the quality of waters in mesotrophic marine ecosystems in which trophic chains are not shortened.

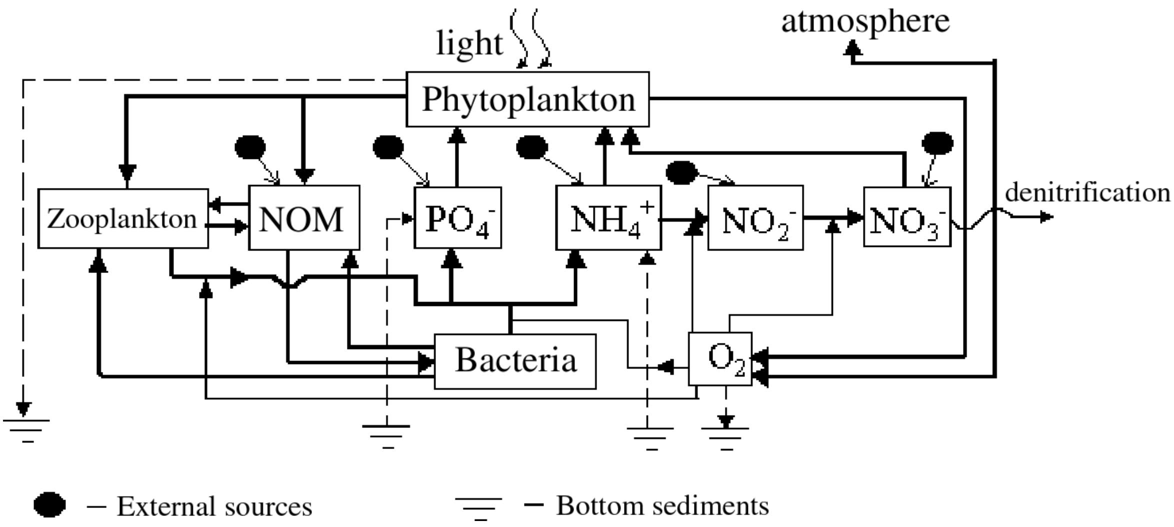


Fig. 4.4. Schematic diagram of relationships between the elements of the block of eutrophication in the model of the quality of waters for the tropical Ciénaga-Grande-de-Santa-Marta Firth.

Including zooplankton in the structure of the block of eutrophication, we assume that its food base is formed by phytoplankton, bacterioplankton, and detritus. Moreover, zooplankton is a strongly aggregated component of actual ecosystems and, hence, it should be taken into account that a part of its organisms (predators) can eat other organisms (phytophagous). The losses of zooplankton for metabolism (respiration) are regarded as the process of regeneration of the mineral compounds of nitrogen and phosphorus and the products of its vital activity, i.e., the nonused remains of food, are included in the pool of inert organic matter [49, 65, 134].

A two-dimensional model of eutrophication whose system of equations is closed on the level of zooplankton was developed and applied by the authors for the tropical shallow-water Ciénaga-Grande-de-Santa-Marta Firth [97, 126]. The mathematical structure of the model is similar to the structure of the model described in the previous subsection (with certain distinctions). The diagram of relationships between the components of the model is presented in Fig. 4.4.

The system of equations of the block of eutrophication taking into account the role played by zooplankton in the formation and variations of the state of an ecosystem is described in what follows.

Phytoplankton, $\mathrm{mgC/m^3}$. We have

$$\left.\frac{dB_f}{dt}\right|_{\mathrm{loc}} = ((1-\gamma_f)\sigma_f(I, C_{\mathrm{PO}_4}, C_{\mathrm{N}}) - \mu_f)B_f - \frac{w_{gf}}{H}B_f - G_1 B_z. \qquad (4.47)$$

Bacterioplankton, $\mathrm{mgC/m^3}$. We have

$$\left.\frac{dB_b}{dt}\right|_{\text{loc}} = \left(V_b^{\max}\frac{B_{\text{org}}}{\Pi_{\text{org}} + B_{\text{org}}}\varepsilon_{\text{ing}} - \mu_b\right)B_b - G_2 B_z. \tag{4.48}$$

Zooplankton, mgC/m^3. We have

$$\left.\frac{dB_z}{dt}\right|_{\text{loc}} = (\eta_1 G_2 + \eta_2 G_2 + (\eta_3 - 1)G_3 + \eta_4 G_4 - \gamma_z - \mu_z)B_z, \tag{4.49}$$

where

$$G_j = V_z^{\max}\frac{p_j B_j}{\Pi_z + \sum_{k=1}^{k=4} p_k B_k}, \quad j = 1,\dots,4, \quad p_j = \frac{\rho_j B_j}{\sum_{n=1}^{n=4}\rho_n B_n},$$

$$p_k = \frac{\rho_k B_k}{\sum_{n=1}^{n=4}\rho_n B_n} \qquad ([34]),$$

$$B_1 = B_f, \quad B_2 = B_B, \quad B_3 = B_z, \quad \text{and} \quad B_4 = \alpha_d B_{\text{org}}.$$

Inert Organic Matter, mgC/m^3. We have

$$\left.\frac{dB_{\text{org}}}{dt}\right|_{\text{loc}} = \mu_f B_f + [(1-\eta_1)G_1 + (1-\eta_2)G_2 + (1-\eta_3)G_3 - \eta_4 G_4 + \mu_z]B_z$$
$$+ \left[\mu_b - \frac{V_b^{\max}}{E}\frac{B_{\text{org}}}{\Pi_{\text{org}} + B_{\text{org}}}\varepsilon_{\text{ing}}\right]B_b + Q_{\text{org}}^{\text{ext}}. \tag{4.50}$$

Phosphorus of Phosphates, mg P/liter. We have

$$\left.\frac{dC_{\text{PO}_4}}{dt}\right|_{\text{loc}} = \left[\left(\frac{1}{E} - 1\right)V_b^{\max}\frac{B_{\text{org}}}{\Pi_{\text{org}} + B_{\text{org}}}\varepsilon_{\text{ing}} B_b + \gamma_z B_z\right.$$
$$\left. - (1-\gamma_f)\sigma_f(I, C_{\text{PO}_4}, C_{\text{N}})B_f\right]\beta_{\text{P/C}}\beta_{\text{m}^3/\text{liter}} + Q_{\text{PO}_4}^{\text{ext}} + Q_{\text{PO}_4}^{\text{sed}}. \tag{4.51}$$

Ammonium Nitrogen, mg N/liter. We have

$$\left.\frac{dC_{\text{NH}_4}}{dt}\right|_{\text{loc}} = \left[\left(\frac{1}{E} - 1\right)V_b^{\max}\frac{B_{\text{org}}}{\Pi_{\text{org}} + B_{\text{org}}}\varepsilon_{\text{ing}} B_b + \gamma_z B_z\right.$$

$$- (\chi - \gamma_f)\sigma_f(I, C_{PO_4}, C_N) B_f \Big] \beta_{N/C} \beta_{m^3/liter}$$

$$- \nu_{N1}\varepsilon_{ing} C_{NH_4} + Q^{ext}_{NH_4} + Q^{sed}_{NH_4}. \tag{4.52}$$

Nitrogen of Nitrites, mg N/liter. We have

$$\left.\frac{dC_{NO_2}}{dt}\right|_{loc} = \nu_{N1}\varepsilon_{ing} C_{NH_4} - \nu_{N2}\varepsilon_{ing} C_{NO_2} + Q^{ext}_{NO_2}. \tag{4.53}$$

Nitrogen of Nitrates, mg N/liter. We have

$$\left.\frac{dC_{NO_3}}{dt}\right|_{loc} = \nu_{N2}\varepsilon_{ing} C_{NO_2} - (1 - \chi)\sigma_f(I, C_{PO_4}, C_N) B_f \beta_{N/C} \beta_{m^3/liter} + Q^{ext}_{NO_3}. \tag{4.54}$$

Dissolved Oxygen, mg O_2/liter. We have

$$\left.\frac{dC_{O_2}}{dt}\right|_{loc} = \Big[(\sigma_f(I, C_{PO_4}, C_N) - \gamma_f) B_f$$

$$- \left(\frac{1}{E} - 1\right) V_b^{max} \frac{B_{org}}{\Pi_{org} + B_{org}} \varepsilon_{ing} B_b - \gamma_z B_z \Big] \beta_{O_2/C} \beta_{m^3/liter}$$

$$- (\beta_{O_2/N1}\nu_{N1} C_{NH_4} + \nu_{N2}\beta_{O_2/N2} C_{NO_2})\varepsilon_{ing} - \frac{Q^{bot}_{O_2} \pm Q^{atm}_{O_2}}{H}. \tag{4.55}$$

where B_{org}, mg C/m^3, is the concentration of inert organic matter (detritus + DOM) suffering biochemical oxidation, α_d is the fraction of detritus in the inert organic matter, B_z, mg C/m^3, is the biomass of zooplankton V_z^{max}, h^{-1}, is the maximum specific rate of consumption of food by zooplankton, γ_z, h^{-1}, is the specific respiration rate of zooplankton μ_z, h^{-1}, is the specific rate of natural mortality of zooplankton, G_j, h^{-1}, are the specific rates of eating of various components of its food base by zooplankton: phytoplankton ($j = 1$), bacteria ($j = 2$), and the detrital part of inert organic matter ($j = 4$) plus the specific rate of cannibalism ($j = 3$), η_j are the coefficients of assimilation of food by zooplankton, ρ_j, ρ_k, p_j, and p_k are the coefficients of selectivity of food in the case of consumption of various types of food by zooplankton, Π_z, mg C/m^3, is a constant of semisaturation with food in the process of growth of zooplankton, Q^{ext}_{org}, $Q^{ext}_{NH_4}$, $Q^{ext}_{NO_2}$, $Q^{ext}_{NO_3}$, and $Q^{ext}_{PO_4}$ are the inflows of allochthonous organic matter and mineral compounds of nitrogen and phosphorus from the external sources (rivers and channels). The remaining notation is similar to that used in Subsection 4.2.

In the described version of the block of eutrophication, the inert organic matter is not separated into the dissolved and detrital parts because the model is constructed for shallow-water basins. However, in analyzing the ration of zooplankton, we take into account solely the detrital part of inert organic matter. It is also assumed that the allochthonous organic matter has the same stoichiometric composition as the autochthonous organic matter because the external sources of organic substances are natural objects. The respiration of phytoplankton and zooplankton is regarded as the process of regeneration of phosphates and ammonium nitrogen.

Conclusions

The mathematical structure of the chemical-and-biological block of the model of the quality of waters is constructed with regard for the possibility of its application to the solution of the problems of self-cleaning and eutrophication of waters.

The problem of self-cleaning is correct for the pollutants that do not have significant natural sources in water media and in the case of modeling of the propagation of pollutants coming to marine media from the local sources of pollution.

As the principal mechanisms of self-cleaning of seawater included in the structure of the model, we can mention the hydrodynamic dilution, (bio)sedimentation, and destruction of pollutants as a result of the integral action of the processes of the chemical and biological nature.

In the block of self-cleaning, we determine the functions of nonconservativeness in Eqs. (1.1) by using the specified or computed destruction coefficients for the investigated pollutants. In view of the diversity of the properties of pollutants and the specific features of their behavior and transformation for various characteristics of the water medium, the form of the functional dependences (or the values of constants) specifying the destruction coefficients for pollutants are set in each case individually, on the basis of the analysis of the literature and experimental data. The existing feedbacks between the modeled variables are neglected in the block of self-cleaning.

Among the applied problems of the ecology of seas solved by using the models of self-cleaning of waters, we can mention the assessment of the level of pollution of marine media by the local sources, the evaluation of the sizes of polluted regions, and the analysis of the role of different sources of pollution in the formation of the quality of marine media.

As the variables of the block of eutrophication, we use the characteristics of the levels of trophicity and saprobity of waters. In this block, we study the biogeochemical cycles of biogenic elements, the processes of production and destruction, and the dynamics of the oxygen content of seawater. Note that it is necessary to attain the balance of substances at every local point of the space with regard for the feedbacks existing between the modeled components of the ecosystem.

The mathematical structure of the block of eutrophication developed for a specific water area of the sea is determined by the character of the solved problems and the amount of the initial data about the object obtained in the course of ecological monitoring. Since the realization of complex ecological monitoring is quite costly, requires significant amounts of time, and imposes high requirements to the available scientific and methodical basis of the complex of necessary observations and experiments, it is reasonable to develop several basic blocks of eutrophication of different levels of complexity (hierarchy) based on different amounts of the initial data.

For this reason, we developed a hierarchy of the blocks of eutrophication with original mathematical structure, different numbers of variables, and different levels of going into details in the description of the relationships between the biotic and abiotic components of the marine ecosystem (model).

The simplest version of the block of eutrophication (first level of the hierarchy) is based on the standard collection of analyzed hydrochemical characteristics (mineral compounds of nitrogen and phosphorus, biochemical oxygen demand, permanganate oxidizability, and dissolved oxygen) and contains a single biotic variable (biomass of phytoplankton) which can be estimated in the first approximation via the concentration of chlorophyll A. The rates of regeneration of the mineral compounds of nitrogen and phosphorus are regarded as equal and described by the kinetic equation of the first-order reaction of biochemical oxidation of the organic matter. The difference between the stoichiometric ratios for the inert organic matter of natural (autochthonous) and anthropogenic origin is taken into account.

In the block of the second hierarchical level developed for the northwest part of the Black Sea, the nitrogen and phosphorus cycles on the abiotic level are studied separately. This enables us to take into account possible differences between the rates of mineralization of the organic compounds of nitrogen and phosphorus and the ratios of nitrogen and phosphorus contents of the autochthonous and allochthonous organic matter (including the substances supplied by the anthropogenic sources). The specific rates of chemical and biological processes are regarded not as constants but as functions of the characteristics of state of the marine medium. The inert organic matter expressed in the units of nitrogen, phosphorus, and oxygen is separated into the suspended and dissolved parts, the first of which undergoes sedimentation under the action of the gravitational forces.

In the block of the third hierarchical level developed for the Cartagena Bay, the role of bacteria in the mineralization of the organic matter is explicitly taken into account, which enables us to give a more exact description of the space and time variability of the modeled characteristics. We propose a new scheme of inclusion of bacterioplankton in the mathematical structure of the model taking into account the influence of density of the population of bacteria on their mortality and the difference between the fractions of biogenic elements in the inert organic matter of natural and anthropogenic origin.

The most complex version of the model of eutrophication (fourth level of the hierarchy) includes both zooplankton and bacteria and can, in fact, be regarded as a simplified version of the model of functioning of water ecosystems.

We also give recommendations concerning the application of all proposed blocks of eutrophication. It is reasonable to use the blocks of the first and second levels for hypertrophic and eutrophic marine ecosystems in which bacterioplankton is adapted to high concentrations of the organic substrate and the trophic chain is shortened. Moreover, the first-level block is intended for the integration in the structure of the two-dimensional (in the space variables) model of the quality of waters and second-level block is used in the three-dimensional model. The block of eutrophication of the third hierarchical level is intended for the integration in the structure of three-dimensional models for water areas of the sea with high levels of saprobity of waters and significant spatial inhomogeneities of the concentration of inert organic matter.

The block of eutrophication of the fourth hierarchical level is used to model the quality of waters in marine ecosystems in which the trophic chains are not shortened and the influence of zooplankton on the dynamics of phytoplankton is significant. Most often, the biomass of zooplankton should be taken into account in modeling the quality of waters in mesotrophic regions of the sea. In the statement presented above, the block is used as a component of the two-dimensional model of the quality of waters. At the same time, the three-dimensional version of the model can easily be constructed on the basis of the block of eutrophication of the third level by using a similar scheme of inclusion of zooplankton in the structure of the model.

The models (blocks) of eutrophication developed and tested for the ecosystems of tropical latitudes can be adapted to the ecosystems of middle latitudes by replacing the constant rates of chemical and biological processes by their functional dependences on the temperature of water.

5. PRINCIPLES AND METHODS OF CALIBRATION OF THE PARAMETERS OF THE BLOCK OF EUTROPHICATION OF THE MODEL OF THE QUALITY OF WATERS

In the course of calibration of the block of eutrophication of the model of the quality of waters, it is necessary to determine the values of the parameters of this block (specific rates of chemical and biological processes) and/or the coefficients of empirical equations used to describe the variations of these parameters depending on the characteristics of the medium and external factors.

As a necessary condition of calibration, we can mention the realization of preliminary ecological monitoring of the investigated water area of the sea in the course of which it is necessary to determine the specific features of variations of the modeled elements of the ecosystem and the natural and anthropogenic factors affecting the behavior of the ecosystem. The problems of organization of the ecological monitoring of water areas of the sea are discussed in Chapter 6 from the positions of mathematical simulation of the processes running in ecosystems.

The main aim of the procedure of calibration is to get the maximum possible agreement between the data of observations and the values of modeled variables computed by using the model both according to the mean statistical values of the parameters and by analyzing the character of their intraannual dynamics. This aim is attained as a result of variation of the parameters of dynamic equations of the model within possible ranges of their variability. For each parameter of the model equations, this range is established in the course of precalibration realized on the basis of the data available from the literature sources.

The procedure of calibration of the parameters of the block of eutrophication for a specific water area of the sea includes the following three stages:

(i) the most probable (typical) values of the parameters included in the equations of the model and their possible ranges under the conditions close to the actual conditions observed in the analyzed marine ecosystem are determined on the basis of the data presented in the scientific literature;

(ii) the values of the most important parameters of the model and the characteristics of production for the biotic variables of the model are determined under the conditions maximally close to the natural conditions in the course of laboratory and *in-situ* experiments;

(iii) the values of the parameters of the model determined in the first stage of calibration are corrected within the admissible ranges of their variation in order to get the maximum possible correspondence between the data of observations and the numerical results.

There are numerous works devoted to the experimental evaluation of the specific rates of principal chemical and biological processes of transformation of substances and energy studied in the models of eutrophication of waters (see, e.g. [12, 63, 81, 109], etc.). However, the conditions of these experiments, methodical bases, media, and the types of investigated hydrobionts are absolutely different. Moreover, each water ecosystem is characterized by its own specific hydrological and hydrochemical conditions, species composition of hydrobionts, structure of trophic links between the species, etc. Therefore, the difference between the characteristics of the same processes obtained by different researchers can be significant. However, it is always possible to select an interval (range) of variations of the analyzed parameter containing the major part of its values experimentally obtained under the conditions close to the conditions typical of the investigated marine ecosystem. This range contains the most probable value of the analyzed parameter used for the purposes calibration of the model as the first approximation to the actual value.

The first stage of the procedure of calibration of the block of eutrophication is based on the analysis of the literature data on the rates of chemical and biological processes. This stage is called the "precalibration" (preliminary calibration) of the model.

For the high-quality calibration of the parameters and coefficients of the model, it is necessary to perform special *in-situ* and laboratory experiments. In the minimum version, the complex of special observations includes the evaluation of the specific production of autotrophs depending on the factors affecting this process and the rates of biochemical oxidation, mineralization of inert organic matter, and gas and mass exchange with the bottom sediments.

The realization of the program of special experiments enables to get the block of eutrophication objectively adapted to the specific conditions of the studied water area, decrease the number of degrees of freedom and uncertainty in the choice of parameters that should be corrected in the third stage of calibration, and hence, increase the reliability of the results obtained by using the model.

The necessity of additional special experiments can also be explained by the impossibility of getting the required balance of substances and energy in the equations of the model in the third stage of calibration by using the values of the parameters of equations established in the stage of precalibration. This situation is most often observed in the case where the conditions of running of certain modeled chemical, biochemical, or biological processes are specific for the analyzed water area.

The entire complex and methodical aspects of special experiments aimed at the evaluation of specific rates of the principal chemical and biological processes studied in the models of eutrophication are described in Chapter 6.

In the third stage of calibration, the primary values of the specific rates of the processes are subjected to variation (within the limits of the established ranges of these parameters) in the course of numerical experiments performed by using the model in order to determine their combinations realizing the main aim of calibration, i.e., guaranteeing the adequacy of the obtained model results to the data of observations.

The general scheme of the third stage of calibration can be described as follows:

On the basis of the data of observations and/or numerical results, we determine the flux of photosynthetically active radiation (PAR) penetrating through the water surface and the empirical relationship between the transparency of water and the factors affecting this quantity (including the parameters of the model). Then we specify the variations of the external factors affecting the behavior of the modeled components of the ecosystem: the quality of waters, the discharge of the anthropogenic sources of pollution and rivers into the analyzed water basin, the hydrometeorological conditions (speed and direction of the wind and air temperature), and the conditions of water exchange with neighboring water areas. These data are used as initial in the numerical experiments carried out by using the model of eutrophication of waters.

As the initial values of the specific rates of chemical and biological processes used in the numerical experiments performed by using the model, we take the most probable values of these quantities established in the process of precalibration.

First, the procedure of calibration is performed for the zero-dimensional (in space) or one-dimensional (in the vertical direction) versions of the model. The zero-dimensional model is used for the precalibration of two-dimensional models of the quality of waters for shallow-water sea basins and the one-dimensional block is used with the three-dimensional models of the quality of waters in deep-water areas of the-sea with significant vertical stratification of the modeled characteristics.

In using the zero-dimensional (point) version of the model, the entire water basin is regarded as a single computational cell (reservoir) whose volume and depth correspond to the volume and mean depth of the actual water basin. The hydrodynamic processes of redistribution of substances over the space are neglected because the model deals with the values of elements of the ecosystem averaged over the volume of the basin. Thus, the model describes solely the local fluxes of substances caused by the chemical and biological processes.

The zero-dimensional version of the model does not contain possible errors of numerical realization of the two-dimensional model and is simpler in operation in the course of numerical experiments aimed at the attainment of the balance of substances in the ecosystem (calibration of the parameters and coefficients of the balance equations). From the viewpoint of validity of the laws of conservation of matter and energy in the ecosystem, the numerical solution of the model equations in the zero-dimensional version is better justified from the mathematical point view than the two-dimensional version.

The preliminary calibration of the one-dimensional version of the model also has some advantages over the three-dimensional version. Thus, in the process of selection and adjustment of the parameters, the one-dimensional model requires much smaller amounts of computer time, which enables us to perform much more numerical experiments with various combinations of parameters of the model and get the required character of variations of the modeled parameters of the quality of waters in the sea or the required balance of the processes of production and destruction under the conditions of invariable external actions.

Note that the application of the zero-dimensional version of the model (model of the photic layer) for the preliminary calibration of the parameters of the three-dimensional model is not recommended because, in this case, the consistency of the results obtained by using versions of the model of different dimensionalities is, as a rule, not preserved due to the significant influence of the method of parametrization of the vertical turbulent diffusion of substances.

In the numerical experiments with zero- or one-dimensional versions of the model, the inflow of substances from the sources external for the modeled ecosystem (river discharge and the sources of anthropogenic origin) is described by the formula [92]:

$$\frac{dC_i}{dt} = Q_i = \sum_k \frac{q_k}{W_{\text{tot}}}(C_i - C_{ki}), \tag{5.1}$$

where Q_i is the rate of changes in the concentration of the i th substance as a result of its inflow from the external sources, q_k is the flow rate of the k th external source of the i th substance, C_{ki} and C_i are, respectively, the concentrations of the i th modeled substance in the waters coming from the k th external source and in the waters of the analyzed basin, and W_{tot} is the total volume of the zone of dilution (the entire volume of the basin in the zero-dimensional version and the volume of a layer of initial dilution in the one-dimensional version).

In the general case, the third stage of calibration of the parameters of the chemical-and-biological block of the model of eutrophication can be realized in the following two ways:

(i) asymptotic calibration; in this case, the procedure of calibration of the model is performed with an aim to get a stable (equilibrium) state of the ecosystem under invariable external conditions corresponding to its actual mean statistical state determined from the data of observations;

(ii) dynamic calibration; in this case, the procedure of calibration is performed to attain the maximum possible correspondence between the dynamics of the components of the ecosystem determined by using the model and according to the data of observations.

The basic idea of asymptotic calibration can be described as follows: We specify the mean statistical values of the external fluxes of substance and energy penetrating into the modeled ecosystem and, for constant values of these fluxes, try to guarantee, as result of numerical calculations according the model, the attainment of a stable state of the ecosystem in which the values of the modeled components correspond to their mean statistical (typical) values determined according to the data of observations. As shown in what follows, this method of calibration proves to be especially efficient for tropical latitudes.

In the procedure of dynamic calibration, the actual variability of external factors specifying the variations of the components of the ecosystem is introduced in the model, and the results obtained by using the model are compared with the data of observations corresponding to given external conditions. It is clear that this type of calibration is most representative because the data of observations are compared not only with the values of the modeled variables but also with their dynamics.

In the course of the third stage of calibration, we perform the analysis of sensitivity of the model to the variations of its parameters and the parameters of external loading. This analysis is performed for each parameter p_k separately and is based on the fact that the range of possible variations of a parameter is established in the stage of precalibration or in the course of special experiments.

One of possible simple procedures of evaluation of the sensitivity of the model can be described as follows:

1. We compute the value of mean relative increment of the parameter p:

$$\Delta x = \frac{p_{\max} - p_{\min}}{p_{\max} + p_{\min}} 100\%,$$

2. Two model experiments are performed for the values $p = p_{\max}$ and $p = p_{\min}$ and fixed (mean) values of the remaining parameters; it is necessary to find the values of response of the model: $S_1 = f(p_{\max})$ and $S_2 = f(p_{\min})$.

3. We compute the relative increment of the analyzed variable of the model S, i.e.,

$$\Delta S = \frac{2|S_1 - S_2|}{S_1 + S_2} \cdot 100\%,$$

As a result, for the k th parameter of the model, we get a couple $(\Delta p_k, \Delta S_k)$ characterizing the sensitivity of the model to this parameter. In a similar way, we can form these couples for all other parameters of the model. They form a set $\{\Delta p_k, \Delta S_k\}$.

The sensitivity of the model to the k th parameter can be estimated by the changes in the mean (for a certain period of time) concentration (biomass) of the variable C_i of the model and the variations of the other statistical characteristics of this variable: its mean square deviation and the maximum and minimum values. Most frequently, the sensitivity of the model of the quality of waters is estimated by analyzing the behavior of the statistical characteristics of variations of the biomass of phytoplankton or primary production of organic matter either for the annual cycle or for the vegetation period. For the tropical latitudes, the sensitivity of the model of eutrophication is estimated according to the values of its variables typical of the stable diurnal course attained in the course of calculations for several decades of the model time.

In [34], the sensitivity of the model is estimated by using a functional of the form

$$J(p) = \frac{E(p) - E_s}{E_s}\left(\frac{p - p_s}{p_s}\right)^{-1}, \tag{5.2}$$

where E_s is the value of a statistical characteristic of the modeled variable in the standard case where the analyzed parameter is equal to p_s and $E(p)$ the value of the same statistical characteristic when the indicated parameter is equal to p.

The accumulated results of evaluation of the sensitivity of the model are used for the determination of the optimal sequence of correction of its parameters in the third stage of the procedure of calibration. On the basis of the analysis of sensitivity, the entire collection of parameters of the model is split into several classes with different degrees of influence on the dynamics of variables of the model. In the course of numerical experiments performed to calibrate the model, we first vary the values of the parameters from the first class whose effect upon the model trajectories is especially pronounced. The values of the remaining parameters established in the stage of precalibration are fixed. The main purpose of variations is to attain the maximum possible correspondence between the model trajectories of the parameters and their actual variability determined according to the data of observations. In this case, the minimized functional has the standard form of the sum of square deviations of the model solution from the experimental curves.

Upon the attainment of certain intermediate results when the subsequent variations of the parameters from the first class do not lead to the improvement of correspondence, we proceed to the variation of parameters from the second class, etc. As soon as a certain optimal collection of values of the parameters of the model is found, we can repeat the procedure of estimation of sensitivity in order to correct the class of the most significant parameters.

The experience of evaluation of sensitivity and calibration of the models of eutrophication for various water areas of the sea [97, 144, 162, 166] shows that the most significant role is played by the parameters of equations of the dynamics of biomass of phytoplankton and the specific rates of biochemical oxidation and mineralization of the inert organic matter. As far as the hydrophysical factors are concerned, the results of calibration strongly depend the intensity of the vertical turbulent diffusion of substances and the rates of gravitational sedimentation of the cells of phytoplankton and detrital particles. For shallow-water areas of the sea, the family of parameters of the first class of significance includes the values of the fluxes of absorption of oxygen by the bottom sediments and the fluxes of biogenic elements directed from the bottom sediments into the bulk of water.

The final correction of the parameters of the model of eutrophication is realized in the course of numerical experiments performed by using the complete two- or three-dimensional versions of the model. To do this, the space distributions of the variables of state of the ecosystem obtained according to the model are compared with the distributions of the same parameters established as a result of observations performed in the course of ecological monitoring.

5.1. Preliminary Evaluation of the Parameters of the Block of Eutrophication (Precalibration)

As shown in Chapter 4, the dependences of the specific rates of chemical and biological processes on the variables of state of the marine medium are described by parametric dependences of different kinds. The determination of the universal complex form of these dependences, typical values of constants (coefficients) appearing in the corresponding relations, and possible ranges of variation of these parameters remains a challenging problem for numerous researchers in the last decades. The generalization of the results obtained by these researchers can be found in [66, 118, 125, 128].

In what follows, we present a brief analysis of the available literature data dealing with the posed problem and corresponding to the stage of precalibration of the block of eutrophication in the model of the quality of waters.

First, we consider the parameters of the equation of dynamics of the biomass of phytoplankton playing the role of the most significant variables in the models of eutrophication of waters in the sea.

Phytoplankton. The maximum specific rate of growth of phytoplankton $V_f^{\max}$, day^{-1}, for a given temperature of water T can be estimated by using the following empirical dependences:

$V_f^{\max}(T) = ab^{cT}$, where $a = 0.6$, $b = 1.066$, and $c = 1.0$ [155];

$V_f^{\max}(T) = \exp(0.0633T - 0.428)$ [66];

$V_f^{\max}(T) = a\exp(0.0725T - 1.135)$, where a varies within the range 1–3 day^{-1} [80];

$V_f^{\max}(T) = V_f^{\max}(20)\theta^{T-20}$ [118], where $V_f^{\max}(20)$ varies within the range 1.4–2.6 day^{-1} and the temperature coefficient $\theta \approx 0.98$–1.072 [167].

For various groups of phytoplankton, the quantity $V_f^{\max}$ can also be estimated on the basis of the data on predominant sizes of the cells, i.e., their volume W_f, μm^3, and surface area S_f, μm^2.

According to [65, 109], $V_f^{\max} = 10^{n/3.32} - 1$, where $n = \tau_f/t_2$ is the number of fissions of a cell per day, τ_f, h, is the photoperiod, and $t_2 = 3.28W_f$ is the characteristic time of doubling of the cells, h.

The dependence of the form $V_f^{\max} = 11.23\,W_f^{-0.266}$ [24] was established on the basis of the data of field studies carried out in the Black Sea for the temperature of water $T \approx$ 16–18°C.

In [132], the following dependences were proposed on the basis of the results of laboratory experiments with cultures of algae:

$$V_f^{\max}(20) = 1.142\left(\frac{S_f}{W_f}\right)^{0.325},$$

$$\log V_f^{\max}(T) = \log V_f^{\max}(20) + b\left[\frac{1000}{273+20} - \frac{1000}{273+T}\right],$$

where

$$b = 3.78 - 2.505\log\left(\frac{S_f}{W_f}\right).$$

In these relations, $V_f^{\max}(20)$ and $V_f^{\max}(T)$ are the maximum growth rates of algae (per day) at the temperatures of water equal to $20°C$ and T, respectively, and S_f, μm^2, is the surface area of the cell.

Constants limiting the process of production of phytoplankton by biogenic elements Π_{PO_4} and Π_N. In [167], one can find the following possible ranges of these parameters of production of phytoplankton in fresh-water ecosystems: $\Pi_N \approx 15–25\,\mu g N/liter$ and $\Pi_{PO_4} \approx 3–20\,\mu g P/liter$. The analysis of numerous literature sources (see, e.g., [12, 65, 66, 76, 83, 118, 125, 128, 129], etc.) performed by the authors shows that the typical values of the constants of semisaturation for phytoplankton in the coastal marine and fresh-water ecosystems suffering eutrophication vary, as a rule, within the following limits: $\Pi_N \approx 14–50\,\mu g N/liter$ and $\Pi_{PO_4} \approx 4–16\,\mu g P/liter$. In this connection, the conclusion made in [74] that the contents of the mineral compounds of nitrogen and phosphorus in water on the following levels: $100\,\mu g N/liter$ and $20\,\mu g P/liter$ are sufficient for the optimal development of various aquatic plants seems to be correct.

Illumination of the water column. The values of the critical and optimal illumination for photosynthesis differ for different types of algae and depend on their living conditions because algae are capable of adaptation to the conditions of illumination. In addition, the models of primary production use two ways of description of the influence of illumination on the photosynthesis of phytoplankton: with and without regard for its photoinhibition under the conditions of redundant illumination. Hence, it is customary to use two different characteristics of illumination: I_k is the illumination corresponding to the onset of saturation with light in the process of photosynthesis and I_{opt} is the illumination for which the rate of photosynthesis is maximum. The quantity I_{opt} should be regarded as the upper limit for which the inhibition of photosynthesis by the redundant illumination is still absent but the state of saturation is already attained. The data of *in-situ* investigations [7, 42] show that the intensity of light optimal for the photosynthesis of phytoplankton (within the range of PAR) in upper layers of the euphotic zone of the ocean is most often equal to 0.03–0.16 cal/cm^2·min (≈ 20–120 W/m^2) or 30–100 cal/cm^2·day and the mean value is equal to 70 cal/cm^2·day. In the relative units, the light optimum constitutes, as a rule, 20–50% of the mean flow of PAR penetrating through the sea surface [65].

In the laboratory experiments with cultures of algae, it is shown that, for the major part of species, the ultimate intensity of light I_k up to which the growth rate of algae is proportional to the intensity of light belongs to the range 0.02–0.25 cal/cm^2·min (15–174 W/m^2) [66, 76, 109]. In the specialized literature, we most often encounter the value $I_k \approx 0.1$ cal/cm^2·min (70 W/m^2). It should be regarded as a reference value in calibrating the models for the entire phytoplankton. For separate systematic groups of algae, it is shown that dinoflagellates exhibit the highest need in elevated values of the intensity of light: $I_k \approx 0.16$–0.20 cal/cm^2·min (112–140 W/m^2). For green (blue-green) algae, the required intensities are minimum: $I_k \approx 0.026$–0.049 cal/cm^2·min (18–34 W/m^2) and the diatoms occupy the intermediate position with $I_k \approx 0.066$–0.12 cal/cm^2·min (46–84 W/m^2) [66, 76]. As shown in [66, 154], the optimal illumination I_{opt} for all groups of algae is higher than I_k by about 0.066 cal/cm^2·min (46 W/m^2).

Generalizing the presented information, we conclude that the optimal levels of illumination I_{opt} typical of phytoplankton lie within the range 60–140 W/m^2.

The rate of gravitational sedimentation w_{gf} of the cells of phytoplankton in seawater can be estimated either by using Stokes' law [27, 66] or on the basis of the data on the predominant size of the cells.

According to Stokes' law, we can write

$$w_{gf} = \frac{g(\rho_f - \rho)d^2}{18\mu\rho}, \tag{5.3}$$

where ρ_f is the density of phytoplankton (≈ 1050–1150 kg/m^3 [17]), ρ is the density of seawater, d is the diameter of cells of phytoplankton, μ is the coefficient of dynamical viscosity of water, and g is the gravitational acceleration.

However, there exists an opinion that the rate of sedimentation of algae depends on the temperature of water to a much greater extent than it follows from Stokes' law. According to [17], the rate of gravitational sedimentation of algae in seawater can be estimated via the characteristic volume of cells of phytoplankton W_f and the temperature of water T by the formula

$$w_{gf} = 0.034\, W_f^{0.25} \exp(0.134T)$$

established in the laboratory experiments. Here, $[W_f] = \mu\text{m}^3$ and $[w_{gf}] = \text{cm/h}$.

In the same work, one can also find the following empirical formula:

$$w_{gf} = 0.144\, W_f^{0.24}.$$

The rate of gravitational sedimentation for the cells of diatoms vary, according to the data presented in [128], by several orders of magnitude within the range 0.1–5 m/day because their buoyancy is indeed a function not only of the parameters of Eq. (5.3) but also of the illumination, concentration of biogenic elements, etc. The mean value of w_{gf} for diatoms ≈ 1 m/day. For the other systematic groups of phytoplankton, the rates of gravitational sedimentation are lower (0.1–0.5 m/day) [128].

The specific rate of respiration of phytoplankton φ_f depends on the temperature of water. Thus, the following empirical formula is used in [118]:

$$\varphi_f(T) = \varphi_f(20)\theta^{T-20},$$

where $\varphi_f(20)$ is the specific rate of respiration at a temperature of 20°C with the range of variation 0.05–0.35 day^{-1} and θ is a temperature coefficient whose values vary within the range 1.045–1.1 [125, 167].

The respiration of phytoplankton is often estimated as a fraction of the gross photosynthesis γ_f equal to 5–25% of the value of P_f [66, 80, 134].

The specific mortality rate of phytoplankton μ_f includes, in the general case, the natural mortality of phytoplankton and the intensity of its eating by zooplankton. The expected values of this quantity may vary within fairly broad limits because the data of laboratory experiments [66] show that even if the specific rate of natural mortality of phytoplankton is studied separately, it depends on the concentration of cells of phytoplankton and may vary from 0.05 to 0.9 day^{-1}. However, in most cases, the natural mortality of phytoplankton is equal to 0.02–0.2 day^{-1} [66, 80, 129, 134] and only in the period of blooming increases to the maximum values.

The fraction of death of phytoplankton caused by its eating by phytophagous organisms can be found in the model (if we consider these organisms as one of the variables of state of the ecosystem) or estimated in the course of special experiments (see Subsection 6.1.3). For this purpose, one can use the following formula proposed in [67]:

$$\mu_{fe} = -\ln\left(1 - \frac{E}{B_f}\right),$$

where μ_{fe}, day^{-1}, is the specific rate of eating of phytoplankton and E and B_f are, respectively, the amount of phytoplankton eaten per day and the biomass of phytoplankton.

Bacterioplankton. The maximum possible specific growth rate of bacteria $V_b^{\max}$ is, as a rule, set equal to 2.0–2.5 day^{-1} [67, 134]. In [67], on the basis of the analysis of the data of *in-situ* observations over the biomass of phytoplankton, the specific growth rate of its cells, and the content of inert organic matter in waters of different levels of trophicity, it is recommended to set the constant of semisaturation Π_{org} for the bacterioplankton of coastal waters equal to $5\text{–}10\ \mathrm{mgO_2/liter}$. The maximum possible biomass of bacteria $B_b^{\max}$ for the open shelf conventionally pure regions of the sea can be estimated as $\approx 1000\ \mathrm{mg/m^3}$. At the same time, for the polluted coastal regions, this quantity can be as high as $\approx 5000\text{–}6500\ \mathrm{mg/m^3}$.

Since the mean value of the coefficient of utilization E of substrate for the growth of bacterioplankton is ≈ 0.33, we have

$$P_b = \frac{R_b E}{1 - E} 0.5 R_b .$$

Thus, the losses for the metabolism (respiration) of bacterioplankton are twice higher than its production. This means that bacterioplankton releases about two thirds of the consumed substrate in the form of the products of metabolism.

Zooplankton. According to the estimates of various researchers [46, 65, 134, 135], the maximum specific growth rate of zooplankton $V_z^{\max}$ varies within the range $0.1\text{–}1.5\ \mathrm{day}^{-1}$, the specific rate of its natural mortality is $\approx 0.01\text{–}0.125\ \mathrm{day}^{-1}$, and the specific rate of release of the products of metabolism is $\approx 0.05\text{–}0.3\ \mathrm{day}^{-1}$. The efficiency of assimilation of food by zooplankton is estimated as varying within the range $60\text{–}75\%$.

Biochemical Transformation of the Inert Organic Matter and Regeneration of the Inorganic Compounds of Biogenic Elements. <u>The specific rate of the hydrolysis of detritus</u> δ under laboratory conditions is $0.04\text{–}0.05\ \mathrm{day}^{-1}$ (see [65, 134]). In the case of separation of detritus into the labile and stable fractions, the specific rates of hydrolysis of these fractions are set equal to 0.075 and $0.005\ \mathrm{day}^{-1}$, respectively [128]. The following dependence is proposed in [80]:

$$\delta = 0.005 \exp(0.1T).$$

<u>The specific rate of biochemical oxidation</u> of the inert organic matter K_{BOD}, day^{-1}, for various temperature conditions can be estimated by using the following empirical relations:

$$K_{\mathrm{BOD}} = 0.042 \cdot 1.072^T \qquad [111],$$

$$K_{\mathrm{BOD}} = 0.054 \exp(0.069(T - 6)) \qquad [5],$$

$$K_{\mathrm{BOD}} = 0.0176 \exp(0.1T) \qquad [18],$$

$$K_{\text{BOD}} = 0.004\exp(0.15T) \qquad [80],$$

$$K_{\text{BOD}} = K_{\text{BOD}}^{20} \cdot 1.047^{T-20},$$

where $K_{\text{BOD}}^{20} = 0.16\text{–}0.23$ [118, 167] is the specific rate of biochemical oxidation for $T = 20°\text{C}$.

The influence of the concentration of oxygen dissolved in water on the rate of biochemical oxidation of the inert organic matter is determined by the constant of semisaturation $\Pi_{O_2} = 0.5\text{–}1\ \text{mg}\,O_2/\text{liter}$ [84, 118, 125, 128].

<u>The specific rates of mineralization</u> of the organic compounds of phosphorus K_{PO_4} and nitrogen K_{NH_4}, day^{-1}, are given by the formulas

$$K_{\text{PO}_4} = a\exp(0.1T), \quad \text{where} \quad a = 0.005\text{–}0.01 \qquad [66],$$

$$K_{\text{PO}_4} = K_{\text{PO}_4}^{20}\,\theta^{T-20}, \quad \text{where} \quad K_{\text{PO}_4}^{20} = 0.1\text{–}0.4, \quad \theta = 1.08\text{–}1.2 \qquad [118, 125],$$

$$K_{\text{NH}_4} = a\exp(0.15T), \quad \text{where} \quad a = 0.004\text{–}0.02 \qquad [66, 80],$$

$$K_{\text{NH}_4} = K_{\text{NH}_4}^{20}\,\theta^{T-20}, \quad \text{where} \quad K_{\text{NH}_4}^{20} = 0.02\text{–}0.2, \quad \theta = 1.02\text{–}1.3 \qquad [118, 125],$$

where $K_{\text{NH}_4}^{20}$ and $K_{\text{PO}_4}^{20}$ are the specific rates of mineralization of the organic compounds of nitrogen and phosphorus at a temperature of $20°\text{C}$.

<u>The specific rates of the process of nitrification</u>, day^{-1}:

first stage: $\quad \nu_{N1} = a\exp(0.1T), \quad \text{where} \quad a = 0.008\text{–}0.012 \qquad [66, 80],$

second stage: $\quad \nu_{N2} = b\exp(0.1T), \quad \text{where} \quad b = 0.04\text{–}0.08 \qquad [66, 80].$

For the total (without separation into stages) specific rate of nitrification ν_{12}, day^{-1}, we get

$$\nu_{12} = \nu_{12}^{20}\,\theta^{T-20}, \quad \text{where} \quad \nu_{12}^{20} = 0.05\text{–}0.15, \quad \theta = 1.08\text{–}1.20, \qquad [118, 125].$$

and ν_{12}^{20}, day^{-1}, is the specific rate of nitrification at a temperature of $20°\text{C}$.

The following absolutely different formula is proposed in [128]:

$$\nu_{N12} = \nu_{N12}^{\max}\frac{C_{\text{NH}_4}}{\Pi_{NIT} + C_{\text{NH}_4}}f(T) \qquad (5.4)$$

where

$$f(T) = \begin{cases} e^{-\varsigma_{NT}(T-T_m)^2}, & \text{for} \quad T \le T_m, \\ e^{-\varsigma_{NT}(T_m-T)^2}, & \text{for} \quad T > T_m. \end{cases}$$

ν_{N12}, $\mathrm{gN/m^3 \cdot day}$, is the rate of nitrification, $\nu_{N12}^{\max}$, $\mathrm{gN/m^3 \cdot day}$, is the maximum rate of nitrification for the optimal temperature of water T_m, Π_{NIT}, $\mathrm{N/m^3}$, is the constant of semisaturation of the process of nitrification relative to the available concentration of ammonium nitrogen, T_m, °C, is the temperature of water for which the rate of nitrification is maximum, and ς_{NT} is a coefficient specifying the influence of temperature on the process of nitrification within the ranges above and below T_m. According to [128], the typical values and ranges of the parameters in the functional dependence (5.4) are as follows: $\nu_{N12}^{\max} = 0.02$–$0.11\ \mathrm{gN/m^3 \cdot day}$, $T_m = 25$–36°C, $\varsigma_{NT} \approx 0.006$, and $\Pi_{NIT} = 0.1$–$3.0\ \mathrm{gN/m^3}$.

The influence of the concentration of oxygen dissolved in water on the rate of the process of nitrification is determined by the semisaturation constant $\Pi_{O_2} = 1$–$2\ \mathrm{mg\,O_2/liter}$ [84, 118, 125, 128].

<u>The specific rate of the process of denitrification</u> υ_{DN}, $\mathrm{day^{-1}}$, is given by the formula

$$\upsilon_{DN} = \upsilon_{DN}^{20}\, \theta_{DN}^{T-20} \left(\frac{\Pi_{DN}}{\Pi_{DN} + C_{O_2}} \right),$$

where $\upsilon_{DN}^{20} = 0.09$–$0.13\ \mathrm{day^{-1}}$, $\theta_{DN} = 1.08$–1.16, and $\Pi_{DN} = 0.1$–$0.5\ \mathrm{mg\,O_2/liter}$ [118, 129].

5.2. Calibration of the Block of Eutrophication in the Model of the Quality of Waters for Ecosystems of Middle Latitudes

The procedure of calibration of the mathematical models of aqueous ecosystems of middle latitudes is, as a rule, performed on the basis of the data of *in-situ* observations over the annual cycle of variations of the hydrometeorological, chemical, and biological parameters of state of the ecosystem. This is explained by the presence of significant seasonal variations of the rates of chemical and biological processes and the flows of substances between the components of the ecosystem depending on the hydrometeorological (temperature of water, river discharge, illumination, character of stratification, etc.), hydrochemical (supply of autotrophs with biogenic elements, conditions of oxidation in the bottom layer, etc.), and hydrobiological (e.g., the succession of phytoplankton) factors. As a result, the trends of development of the ecosystem and the ratio of intensities of the processes of production and destruction in the system permanently vary during a year.

Thus, we can speak about stationary states of aqueous ecosystems described by a mathematical model and the corresponding balance of the processes of production and destruction only on the scale of annual cycles.

For this reason, the procedure of calibration of the blocks of eutrophication in the models of the quality of waters for ecosystems of middle latitudes is performed by comparing the model and observed curves of the annual course of the variables of state of the ecosystem.

We illustrate the procedure of calibration by using, as an example, the model of eutrophication of the Dnieper-Bug estuary region and the Odessa region of the northwest part of the Black Sea (see Subsection 2.2.1).

As basic parameters, we used the values of coefficients and parameters of the CE-QUAL-ICM and WASP5 models [118, 128]. The procedure of correction of these parameters within the allowable intervals of their variation was realized by comparing the curves of intraannual variability of elements of the ecosystem obtained by using the model with the average (over the space) data of ecological monitoring of the Odessa region in the northwest part of the Black Sea carried out by the Odessa Branch of the Institute of Biology of Southern Seas in 1988–1999.

The intraannual dynamics of modeled elements of the ecosystem is determined by the seasonal variability of temperature and transparency of waters and the flow of photosynthetically active solar radiation. The temperature of water is one of the variables of the hydrodynamic block and is computed in the model. The transparency of waters is expressed via the integral coefficient Z_d of attenuation of light with depth α by the formula $\alpha = 2.3/Z_d$ [139]. In the model, the coefficient α is represented in the form of a sum of two terms as follows: $\alpha = \alpha_s + \alpha_f$, where α_s and α_f are, respectively, the components taking into account the contributions of the allochthonous suspension and phytoplankton (self-shadowing) to the attenuation of the flow of photosynthetically active solar radiation.

Since mineral suspensions come to the sea with river discharge, it is natural to assume that the salinity of the surface layer of seawater in the investigated region and the concentration of mineral suspension in water are correlated parameters. On the basis of the analysis of the data of observations and literature sources [14], we propose the following empirical formula $Z_d = 0.157\exp(0.233S)$, where S is the salinity of water in the surface layer. By using this formula and the values of salinity computed according to the model, the values of α_s were found at each point of the computational region. In order to compute α_f, we used the following empirical formula [11]: $\alpha_f = 0.18\,B_{f,\mathrm{chl.A}}^{0.395}$, where $B_{f,\mathrm{chl.A}}$, mg chl.A/m^3, is the biomass of phytoplankton. The seasonal variability of the optimal (for photosynthesis) illumination was specified according to the empirical relation $I_{\mathrm{opt}} = 17.0\exp(0.066T)$, W/m^2, where T is the temperature of water.

The evaluation of the parameters of flow of short-wave radiation penetrating through the water surface was realized on the basis of the daily average data of observations over the relative humidity of air and cloudiness carried out at the Geophysical Observatory of the Odessa State Ecological University according to the procedure proposed in [150] and described in Subsection 3.1.4.

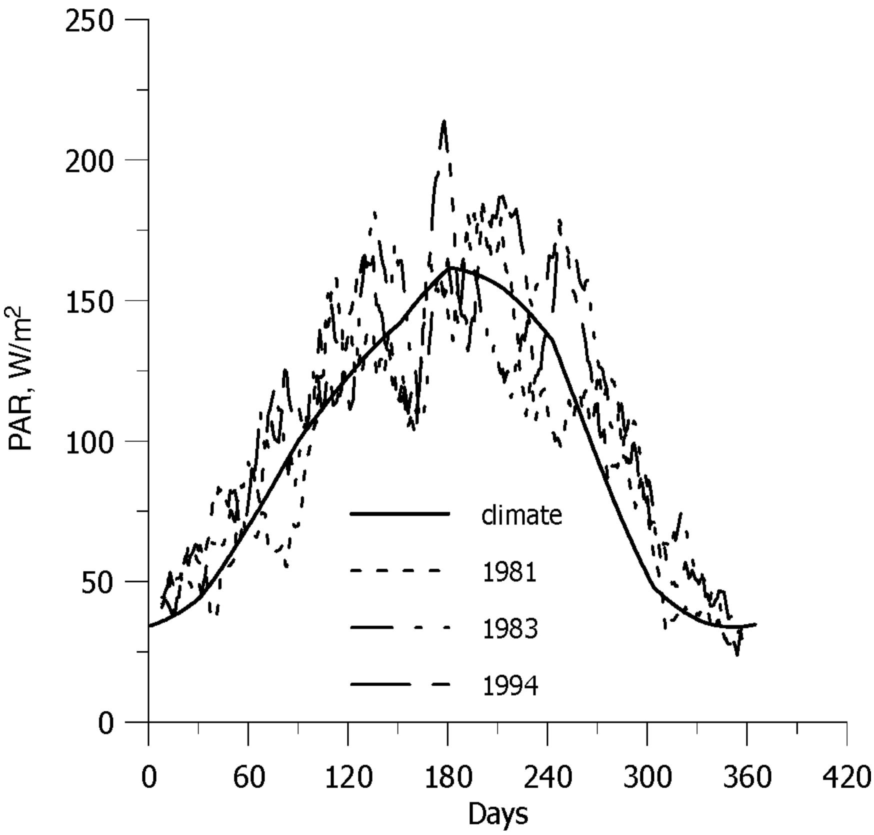


Fig. 5.1. Annual course of the intensity of PAR, W/m^2, averaged over the daytime and computed by using the model for different years and mean climatic conditions.

The same procedure was used to estimate the duration of the daytime. It was assumed that PAR constitutes 50% of the total flow of radiation. The results of calculations are presented in Figs. 5.1 and 5.2.

First, the calibration of parameters of the block of eutrophication was carried out on the basis of the data of *in-situ* observations for a one-dimensional (along the vertical) version of the model (see Subsection 3.4). The main aim of calibration was to attain the required correspondence between the orders of the values of elements of the ecosystem established as a result of observations and obtained in the course of modeling and the specific features of their intraannual variability in the photic layer. This program was realized by correcting, within the allowable limits, the initial values of constants of the block of eutrophication specified according to the literature data.

In order to take into account the supply of biogenic substances by the river discharge and the waste waters of coastal anthropogenic sources, relation (5.1) was used in the one-dimensional version of the model. It was assumed that the dilution occurs inside the upper 10-m layer. In analyzing the contribution of the coastal anthropogenic sources, the horizontal sizes of the zone of dilution were limited by the boundaries of the Odessa region in the northwest part of the Black Sea. For the river discharge, the corresponding zone included the entire computational region of the Dnieper–Bug estuary basin, including the Odessa region (Fig. 3.4).

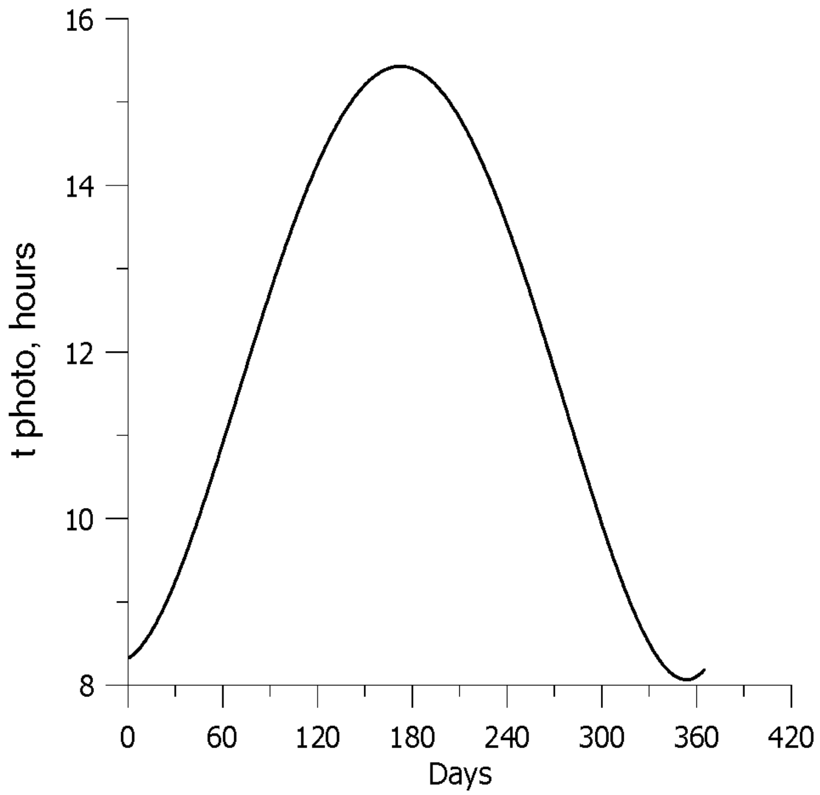


Fig. 5.2. Seasonal variations of the duration of daytime (photoperiod) in hours computed according to the model.

For the purposes of computations, we used ten different levels in depth in the σ-coordinate system. The time step of the chemical-and-biological block was set equal to 1 day. In the course of computations, we assimilated the data of regular 6-h observations over the air temperature, speed and direction of the wind, and the intensity of PAR averaged over the daytime. The numerical analysis was carried out with regard for the seasonal variations of the vertical distribution of salinity caused by the variations of discharge of the Dnieper and Yuzhnyi Bug Rivers (see Subsection 3.4).

The procedure of calibration of parameters of the model was realized according to the following program: First, the annual course of the concentrations of mineral compounds of nitrogen and phosphorus and dissolved oxygen was specified on the basis of the data of observations. Then the parameters and coefficients of the equations for the biomass of phytoplankton, the concentrations of organic compounds of nitrogen and phosphorus, and BOD were varied with an aim to get the maximum possible correspondence between the model curves and the observed values. After this, the system was consecutively supplemented with the equations for the mineral compounds of nitrogen and phosphorus. Finally, the equation of balance of dissolved oxygen was added to the system. It should be emphasized that the parameters of the model are corrected in each stage of the procedure.

Note that the proposed scheme of calibration reflects the contributions of separate elements of the ecosystem and chemical and biological processes described in the block of eutrophication to the variations of state of the analyzed ecosystem.

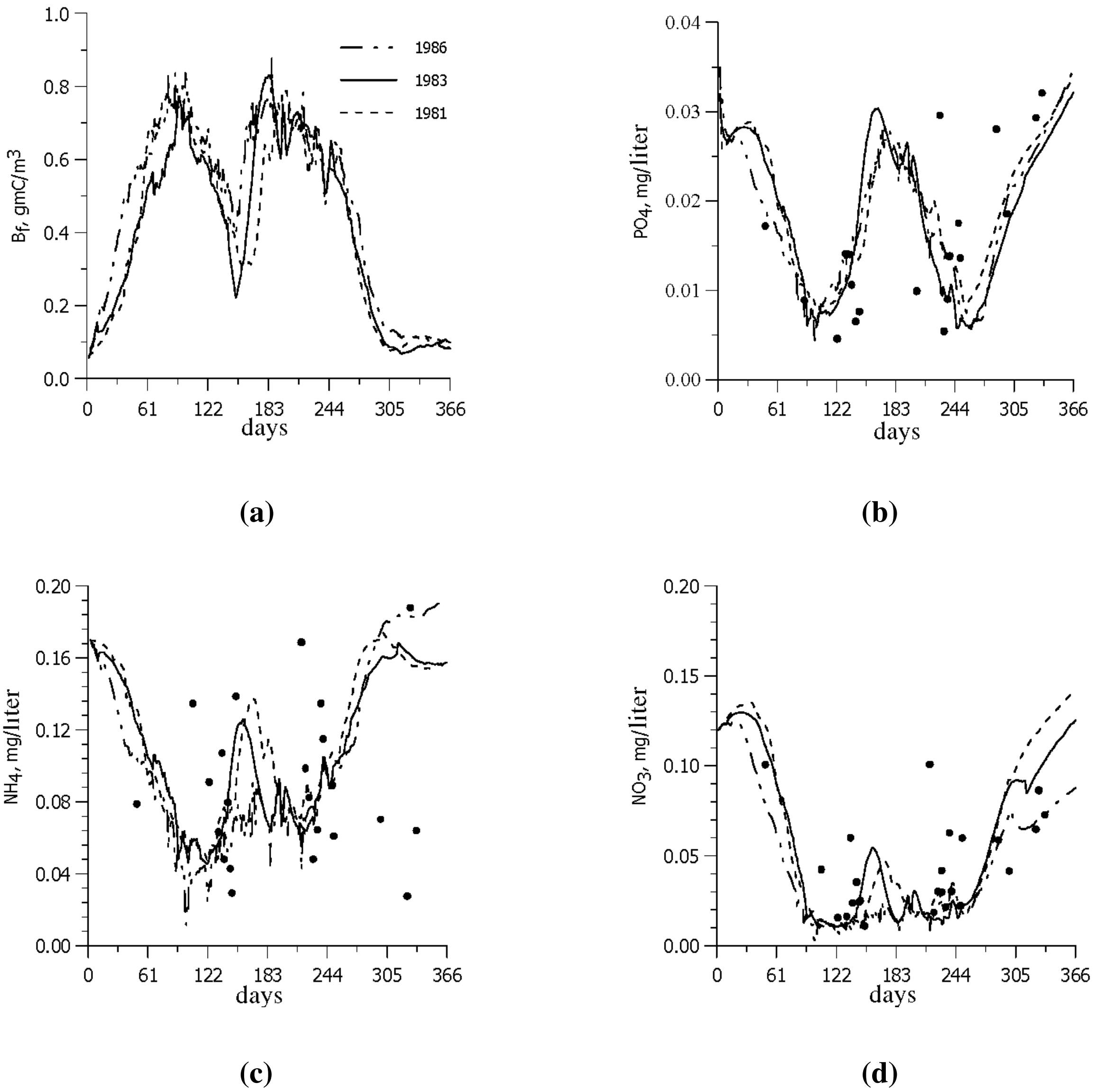


Fig. 5.3. Annual cycles of: (a) the biomass of phytoplankton, g C/m^3, (b) the concentration of phosphorus of phosphates, mg P/liter, (c) the concentration of ammonium nitrogen, mgN/liter, and (d) the concentration of nitrogen of nitrates, mg N/liter, in the surface layer of the Odessa region in the northwest part of the Black Sea computed by using a one-dimensional version of the model of eutrophication. The symbols mark the data of observations obtained in the course of ecological monitoring of the Odessa region in 1988–1999 and averaged over the area of the test range.

The models of eutrophication of waters proposed for the water basins located at tropical latitudes were calibrated by using the same scheme.

The results of calibration of the parameters of the one-dimensional version of the model are presented in Figs. 5.3 and 5.4. The numerical analyses were carried out for the meteorological conditions of 1981, 1983, and 1986. In modeling of the dynamics of phytoplankton according to data from [18, 26, 70, 75], it is assumed that the annual course of the biomass of phytoplankton has two maxima (in March–April and July–August) with peak values of up to 8–16 g/m^3 (wet weight) or 0.4–0.8 g C/m^3.

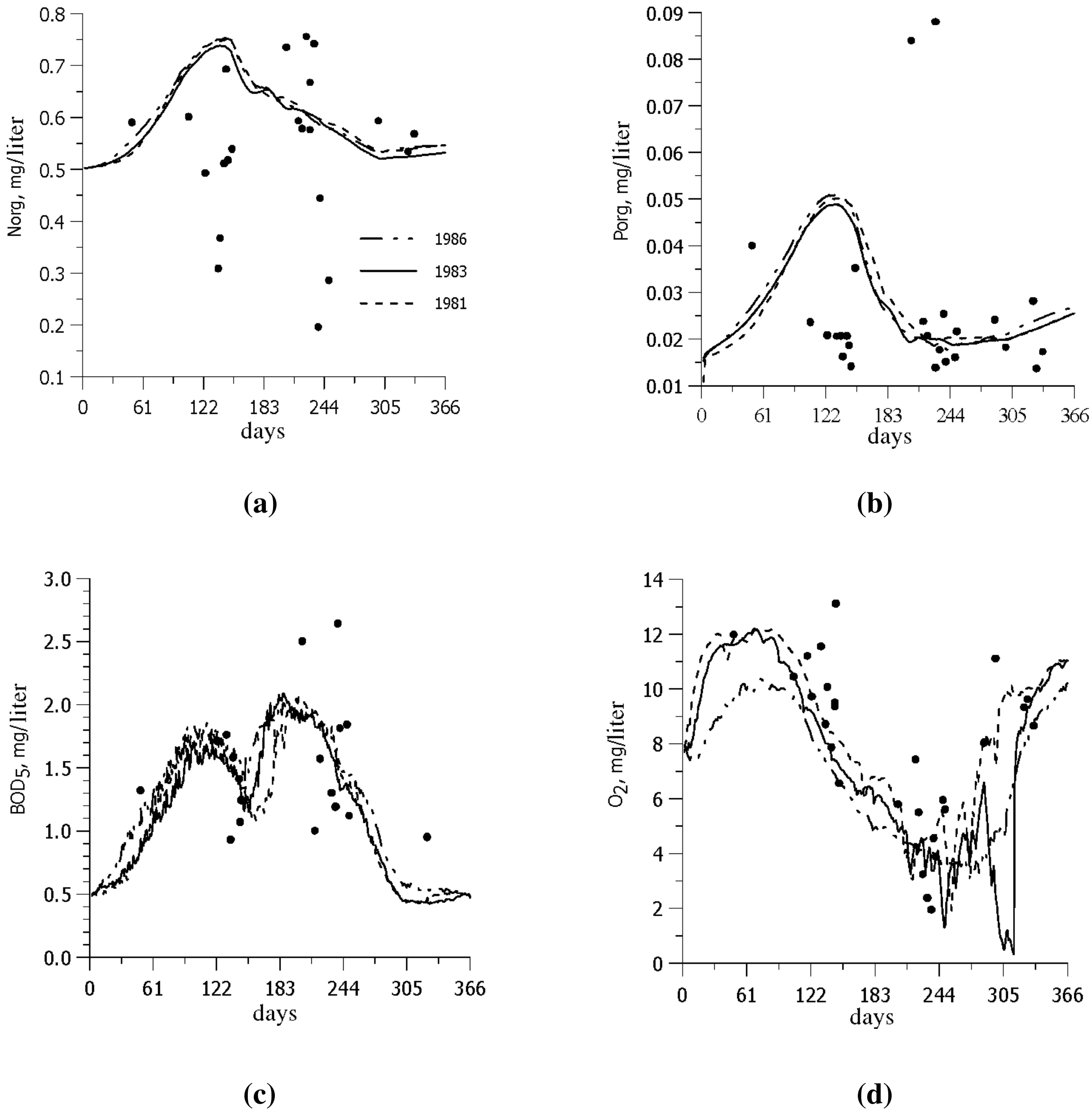


Fig. 5.4. Annual cycles of: (a) the concentration of organic nitrogen, mgN/liter, (b) the concentration of phosphorus, mgP/liter, (c) BOD_5, mg O_2 /liter, in the surface layer, and (d) the concentration of oxygen, mg/liter, in the bottom layer of the Odessa region in the northwest part of the Black Sea computed by using a one-dimensional version of the model of eutrophication. The dark symbols mark the data of surveys carried out in 1988–1999 and averaged over the area of the test range.

The minima of biomass are expected in December–January and in May.

The improvement of the values of some constants was performed in the course of numerical experiments with the three-dimensional version of the model. The parameters and coefficients of the model accepted after its calibration are presented in Table 5.1.

The accumulated numerical results show that the influence of the discharge of Rivers Dnieper and Yuzhnyi Bug on the productivity of waters in the analyzed water area is predominant.

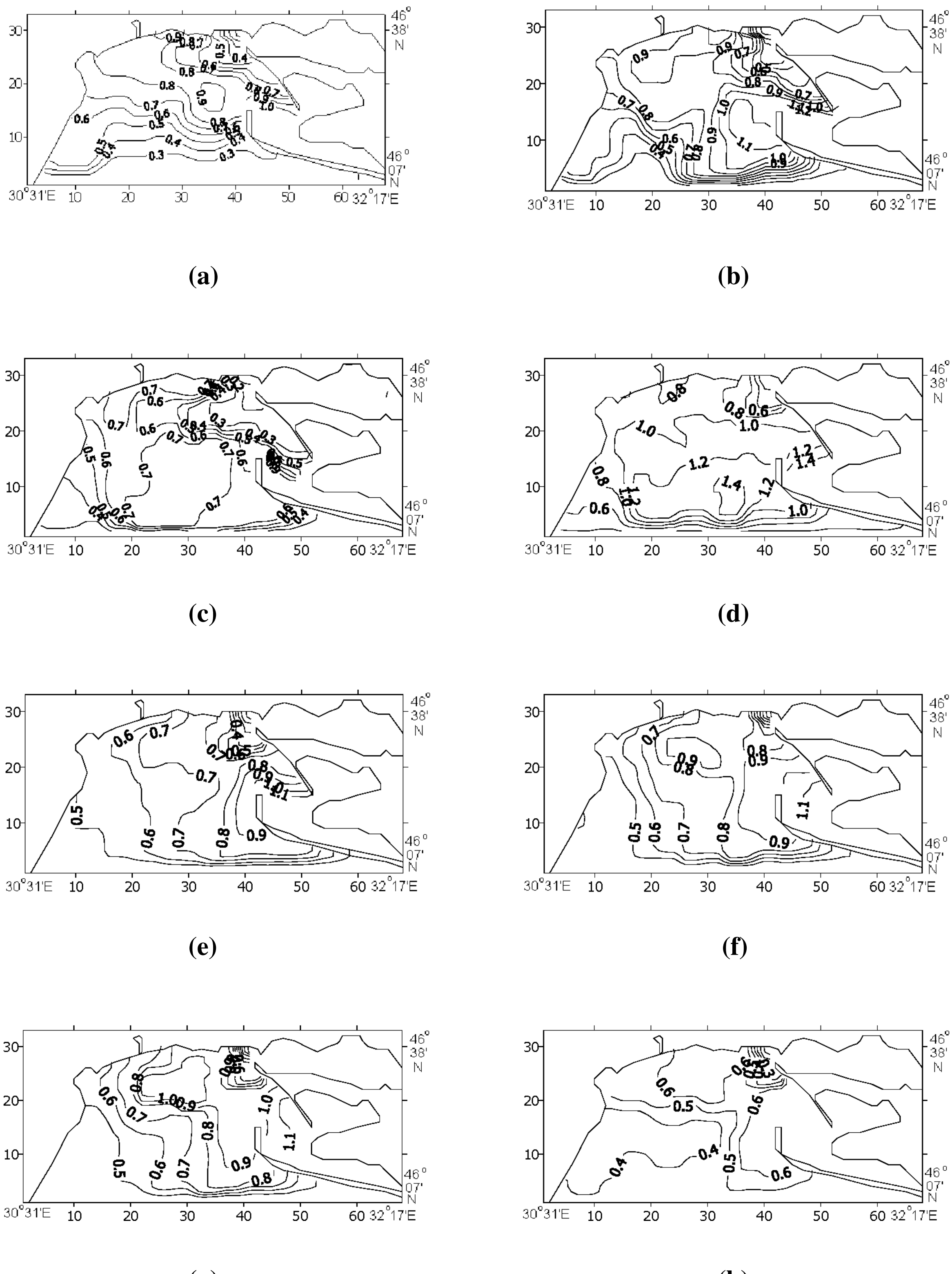


Fig. 5.5. Space distributions of the biomass of phytoplankton, $\mathrm{g\,C/m^3}$, in the surface layer computed by using the model for the meteorological conditions of 1986 corresponding to the following dates: (a) April 14 (b), May 4, (c) May 24, (d) June 20, (e) June 30, (f) July 25, (g) August 9, (h) August 30.

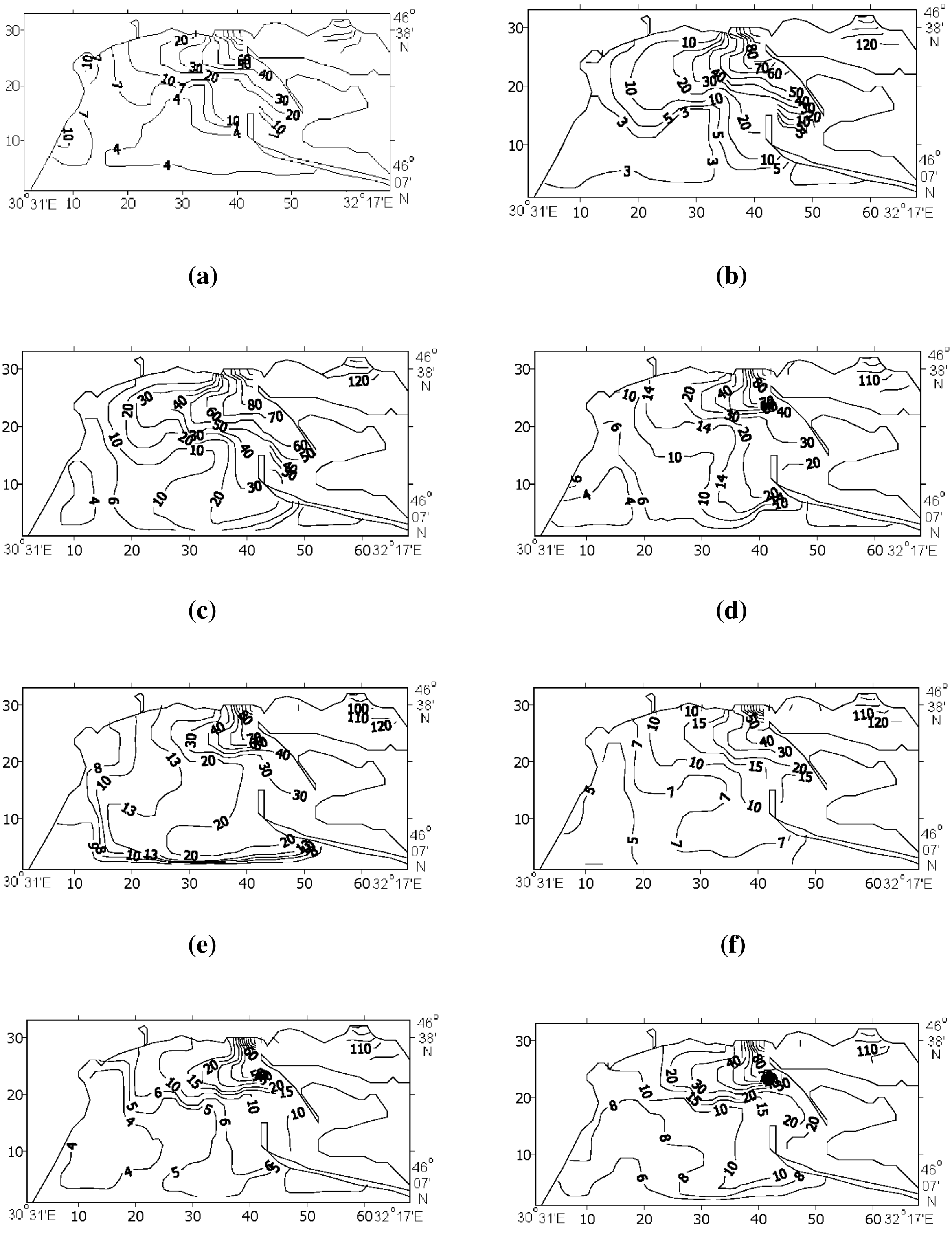


Fig. 5.6. Space distributions of the concentrations of phosphates, μgP /liter, in the surface layer computed by using the model for the meteorological conditions of 1986 corresponding to the following dates: (a) April 14 (b), May 4, (c) May 24, (d) June 20, (e) June 30, (f) July 25, (g) August 9, (h) August 30.

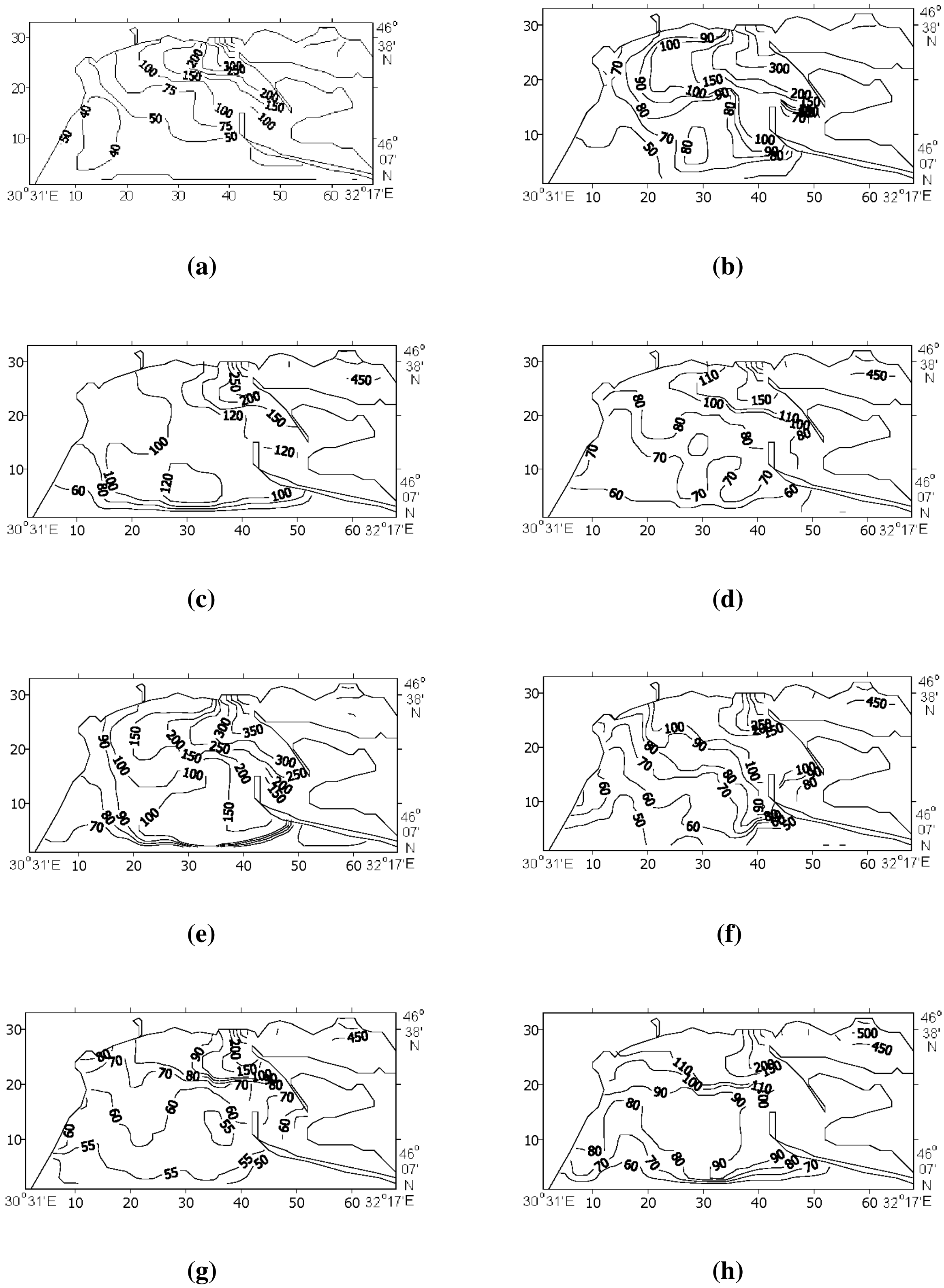


Fig. 5.7. Space distributions of the concentrations of ammonium nitrogen, μg N/liter, in the surface layer computed by using the model for the meteorological conditions of 1986 corresponding to the following dates: (a) April 14 (b), May 4, (c) May 24, (d) June 20, (e) June 30, (f) July 25, (g) August 9, (h) August 30.

Table 5.1. Values of the Parameters and Coefficients of the Block of Eutrophication of the Model of the Quality of Waters in the Northwest Part of the Black Sea Accepted After Calibration

Parameter	Value	Units	Parameter	Value	Units
$V_f^{\max}$	2.25 (2.0)[1]	1/day	g_{N1}	0.	—
ς_1	0.008 (0.004)[1]	$1/{}^\circ C^2$	g_{N2}	0.65	—
ς_2	0.010 (0.006)[1]	$1/{}^\circ C^2$	g_{N3}	0.3	—
T_m	25. (10.)[1]	°C	$\upsilon_{NO_3}^{20}$	0.1	1/day
Π_N	0.050	gN/m^3	Π_{DN}	0.09	$g\,O_2/m^3$
Π_{PO_4}	0.005	gP/m^3	θ_{DN}	1.09	—
φ_r	0.1 (0.08)[1]	1/day	δ_N^{20}	0.03	1/day
T_r	25.	°C	g_{C2}	0.6	—
ς_φ	0.069	1/°C	g_{C3}	0.3	—
μ_r	0.10 (0.22)[1]	1/day	δ_c^{20}	0.03	1/day
ς_μ	0.069	1/°C	θ_c	1.1	—
w_{gf}	0.1	m/day	K_{BOD}^{20}	0.16	1/day
$\beta_{P/C}$	0.022	gP/gC	θ_{BOD}	1.16	—
α_P	0.	—	$\beta_{O_2/DN}$	2.86	$g\,O_2/gN$
$K_{PO_4}^{20}$	0.14	1/day	$\beta_{O_2/C}$	2.67	$g\,O_2/gC$
θ_{PC}	1.1	—	$\beta_{O_2/NT}$	4.57	$g\,O_2/gN$
Π_C	0.6	gC/m^3	ζ_e , ζ_i	22.0, 11.5	$liter/m^2h$
g_{P1}	0.	—	$Q_{O_2}^{T_b}$	– 3.5	$g\,O_2/m^2day$
g_{P2}	0.5	—	ς_o	0.07	1/°C
g_{P3}	0.3	—	T_b	8.0	°C
δ_P^{20}	0.03	1/day	$Q_{NH_4}^{br}$	0.05	gN/m^2day
θ_{par}	1.1	—	$Q_{PO_4}^{br}$	0.005	gP/m^2day

Parameter	Value	Units	Parameter	Value	Units
$\beta_{N/C}$	0.205	gN/gC	ς_{ci}	0.07	1/°C
α_N	0.	—	T_{br}	20.	°C
$K^{20}_{NH_4}$	0.06	1/day	k_{sw}	0.2	m/day
θ_{NC}	1.08	—	ς_{dn}	0.07	1/°C
ν^{20}_{12}	0.04	1/day	$T_{r\,NO_3}$	20.0	°C
θ_{NIT}	1.16	—	$w_{g\,POP}$	0.5	m/day
Π_{NIT}	0.5	gN/m^3	$w_{g\,PON}$	0.5	m/day
Π_{O_2}	1.0	$g\,O_2/m^3$	$w_{g\,det}$	0.5	m/day

Comment: 1. The value of the parameter corresponding to the spring period (March–May).

The maximum biomasses of phytoplankton correspond to the regions of the Odessa Bank and the north end of the Tendrovkaya Spit. In the Odessa region, the maximum biomasses of phytoplankton in the spring–summer period are recorded in the north part of its water area. The elevation of the concentrations of biogenic elements in the photic layer is visually traced near the coast. This elevation is caused by functioning of the coastal anthropogenic sources (see, e.g., Figs. 5.6a, d, h and 5.7f, g, h). The indicated regularities are confirmed by both the literature data [60, 69, 71] and the results of ecological monitoring carried out by the Odessa Branch of the Institute of Biology of Southern Seas (see Subsection 2.2.1) [70, 106].

In Figs. 5.5–5.7, we present some results of modeling of the variations of the space distributions of phosphates, ammonium nitrogen, and the biomass of phytoplankton in the surface layer of the Odessa and Dnieper–Bug regions in the northwest part of the Black Sea obtained by using the three-dimensional version of the model for the hydrometeorological conditions (air temperature and winds) of 1986.

5.3. Calibration of the Blocks of Eutrophication in the Models of the Quality of Waters for Ecosystems of Tropical Latitudes

At the tropical latitudes, the annual cycle of variations of the hydrometeorological factors (temperature of water, PAR, etc.) affecting the state of ecosystems is very weakly pronounced. Moreover, its amplitude is comparable with the amplitude of their short-term variations (for about several days). Therefore, the daily average values of the chemical and biological variables of state of the ecosystem are characterized by much smaller deviations from their annual average values characterizing their stationary state than at middle latitudes. The balance of the processes of production and destruction in the ecosystem is attained not on the annual scale as at middle latitudes but for time periods of several days. Hence, the characteristics of stationary states of the ecosystems of tropical water basins can be obtained as a result of averaging of the data of observations corresponding to various time periods of the annual cycle. The values of the variables of state of the ecosystem obtained as indicated above are called typical or characteristic.

All these arguments enable us to conclude that the main aim of calibration of the models of eutrophication of tropical water areas of the sea is to get, as a result of numerical analysis under annual average hydrometeorological conditions and invariable external loads, a stationary state of the ecosystem characterized by the attainment of the daily average values of modeled variables corresponding to their typical values obtained as a result of time averaging of the data of observations.

On the other hand, at tropical latitudes, the daily cycle of variations of the chemical and biological parameters of the quality of waters is well pronounced and often predominant, which is explained by high rates of production and biochemical oxidation of the organic matter. Therefore, the stationary state of the ecosystem is characterized, parallel with the attainment of the daily average values of modeled variables, by the realization of their diurnal cycle, i.e., by the diurnal balance of the processes of production and destruction.

In view of this observation and the fact that the investigated tropical marine ecosystems are formed in water basins of tidal type whose current dynamics strongly depends on the phase of a tide, the time step of the models of eutrophication for these water areas is set equal to 1 h.

5.3.1. Calibration of the Model of the Ciénaga-de-Tesca Lagoon

Since the analyzed lagoon is a shallow-water basin, we used a two-dimensional modification of the model (without resolution in depth).

In the stage of precalibration, the parameters of the model were reduced to a temperature of water of 30°C [162] with the help of the empirical relations presented in Subsection 5.1.

On the basis of the results of correlation analysis of the data of ecological monitoring, we deduced the following empirical dependence of the attenuation coefficient of light in waters of the lagoon α, m^{-1}, on the concentration of chlorophyll A (Fig. 5.8):

$$\alpha = 2.54\, B_{\mathrm{chl.A}}^{0.34},$$

where $B_{\mathrm{chl.A}}$, mg chl. A/m^3, is the biomass of phytoplankton.

The calibration of the local (zero-dimensional) version of the model was realized in the asymptotic and dynamic modes.

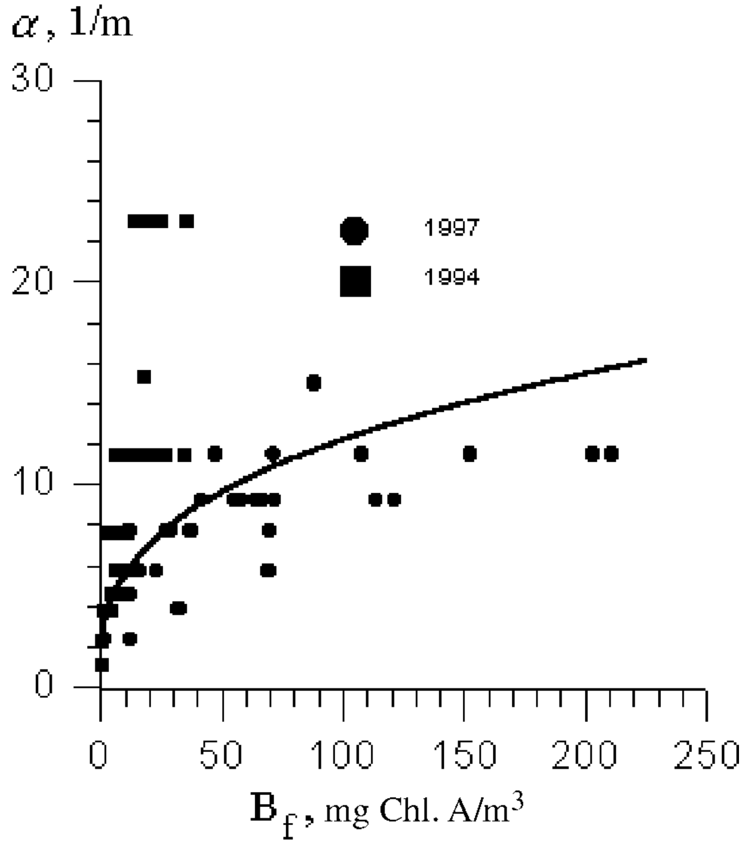


Fig. 5.8. Dependence of the extinction coefficient of light α, 1/m, on the biomass of phytoplankton $B_{\text{chl.A}}$, mg chl.A/m^3, for the Ciénaga-de-Tesca Lagoon. The dark symbols mark the data of observations and the curve corresponds to the approximation accepted in the model.

In the first stage, we determined the family of parameters and coefficients for which the trajectories of variables modeled under the annual average conditions of illumination and invariable anthropogenic loads approach the stationary state (Fig. 5.9) in which the daily cycles of modeled variables are stabilized on the levels corresponding to their typical values established as a result of time averaging of the data of ecological monitoring (see Subsection 2.1.2). Moreover, in order to take into account the contribution of anthropogenic sources to the formation of hydrochemical conditions in the Ciénaga-de-Tesca Lagoon, we use relation (5.1), where W_{tot} is the total volume of waters in the lagoon.

In Fig. 5.10, we present the results of calibration of the model according to the daily course of the concentration of dissolved oxygen and the requirement of attainment of the daily balance in the processes of production and destruction as the system approaches its stationary state.

In the second stage, to check the quality of calibration of the model performed in the asymptotic mode (by analyzing the daily course) on the scales of seasonal and interannual variations, we perform the independent analysis of the dynamics of modeled elements of the ecosystem for two years (1996–1997) for the variable values of the intensity of illumination computed according to the data of daily observations over the humidity of air and the cloud amount (Fig. 5.11).

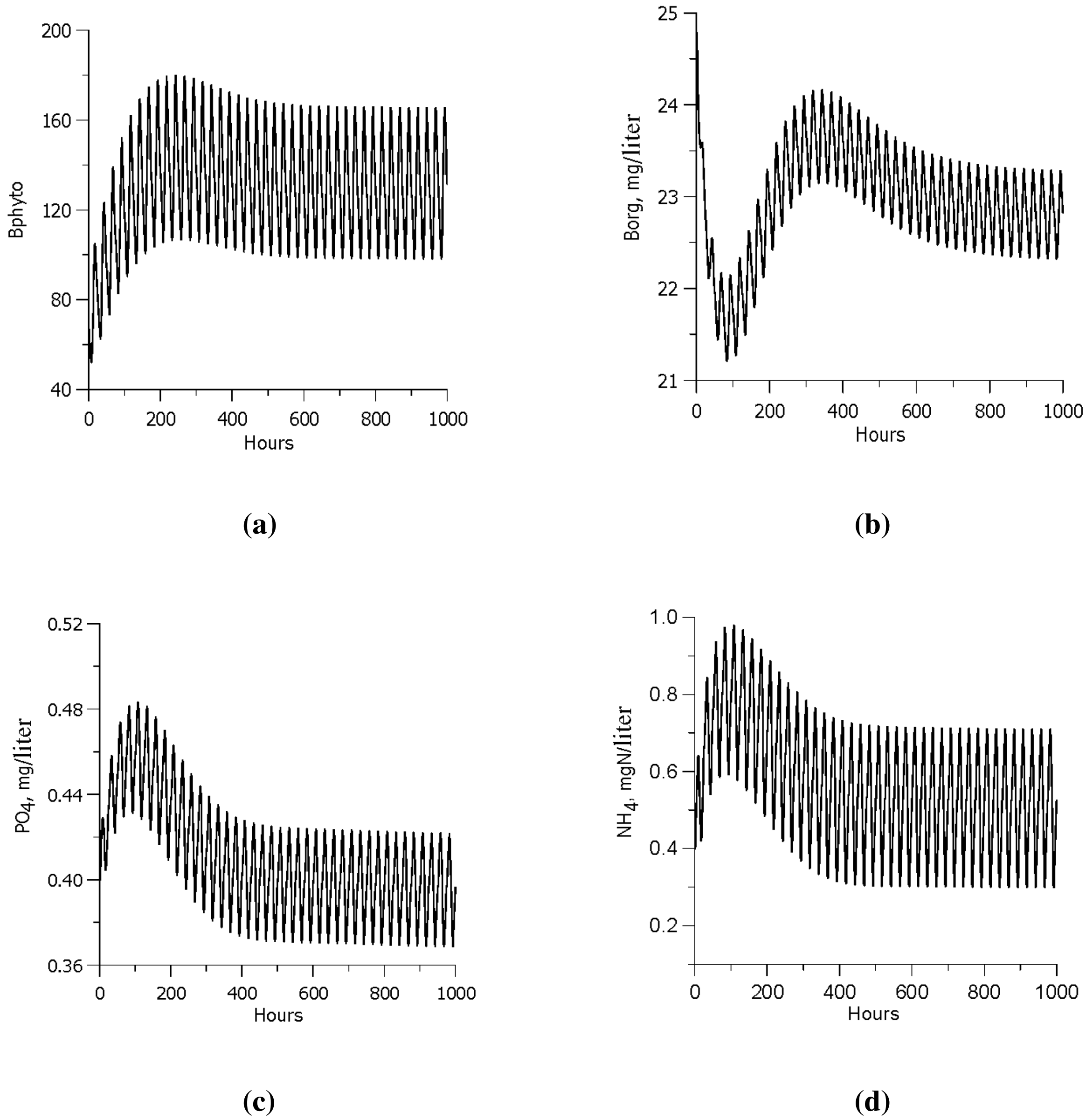


Fig. 5.9. Dynamics of transition of the analyzed variables into a stationary mode (dry season) for the asymptotic calibration of the model of eutrophication of waters of the Ciénaga-de-Tesca-Lagoon: (a) biomass of phytoplankton, mg chl. A/m^3, (b) inert organic matter, mg O_2 /liter, (c) phosphorus of phosphates, mg P/liter, (d) ammonium nitrogen, mg N/liter.

The results of calculations are presented in Fig. 5.12.

The model values of the hydrochemical characteristics of the ecosystem for the corresponding times were compared with the values of these characteristics measured in the course of hydrochemical surveys in 1996–1997 and averaged over the water basin. As follows from Fig. 5.12, the level of agreement between the model and observed values is quite high, especially if we take into account the fact that the water exchange of the Ciénaga-de-Tesca Lagoon with the sea and the seasonal variability of the components of water balance were neglected in these calculations.

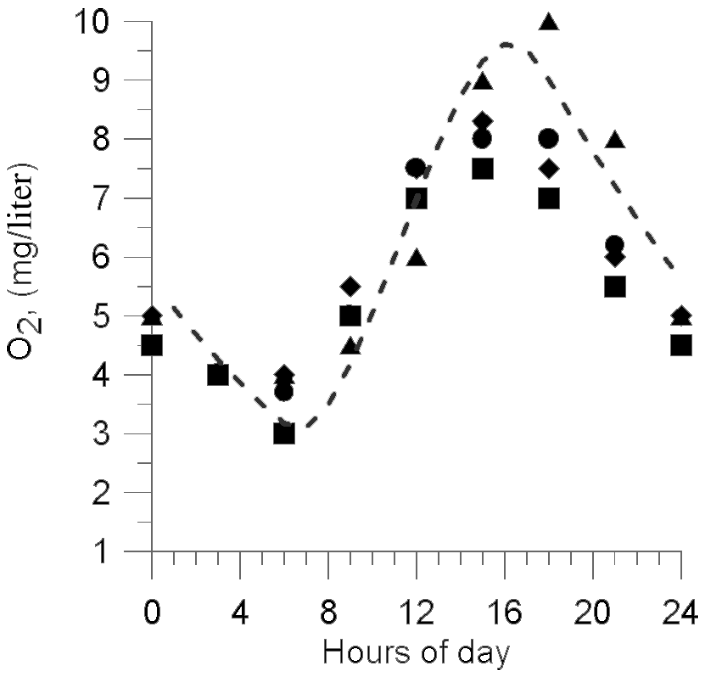


Fig. 5.10. Daily course of the concentration of oxygen, mg/liter, in waters of the Ciénaga-de-Tesca Lagoon plotted according to the data of observations at various points of the water area (symbols) and computed according to the model.

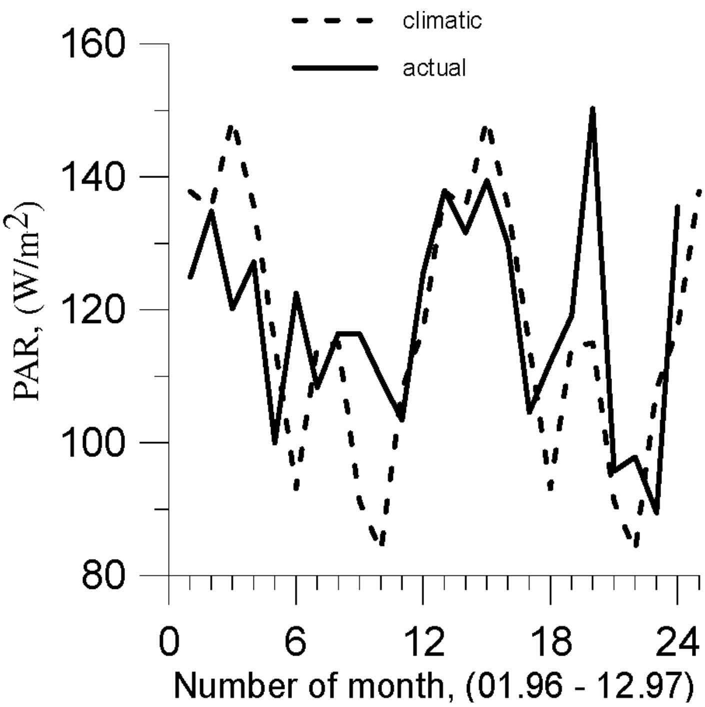


Fig. 5.11. Variations of the average (over the daytime) PAR penetrating through the water surface, W/m^2, reproduced by the model according to the monthly average data of meteorological observations carried out in 1996–1997 (solid line) and according to the many-year average data for the Cartagena Harbor (dashed line).

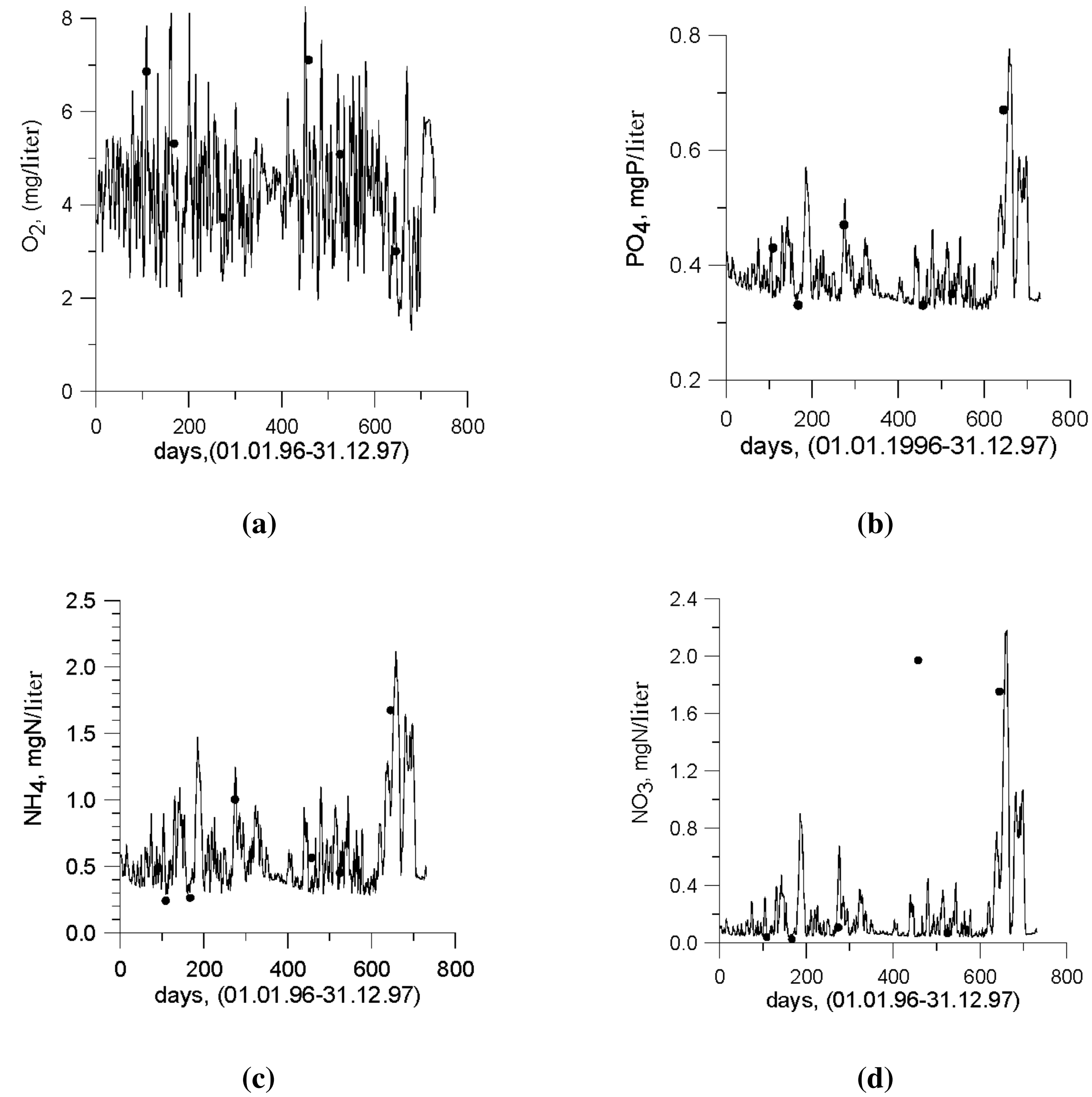


Fig. 5.12. Variations of the concentrations of: (a) oxygen, mg/liter, (b) phosphates, mgN/liter, (c) ammonium nitrogen, and (d) nitrates, mg/liter, in the Ciénaga-de-Tesca Lagoon for two years computed according to the zero-dimensional version of the model for 11.00 of each day (solid lines) and obtained as a result of averaging of the data of observations (symbols) over the space for the corresponding times.

Thus, the calibration of the zero-dimensional version of the model shows that this model enables us to give an adequate description of variations of the principal chemical and biological parameters of the quality of waters in the ecosystem of the lagoon with a degree of accuracy sufficient for the practical purposes.

The final calibration was carried out for the two-dimensional version of the model by comparing the model and observed space distributions of elements of the ecosystem and required small correction of the values of constants determined in the numerical experiments with the zero-dimensional version. The values of constants of the block of eutrophication accepted after the procedure of calibration are presented in Table 5.2.

Table 5.2. Values of Constants of the Block of Eutrophication of the Model of the Quality of Waters in the Ecosystem of the Ciénaga-de-Tesca Lagoon Obtained as a Result of Its Calibration

Parameter	Value	Units	Parameter	Value	Units
V_f^{max}	4.0	1/day	$\beta_{P/C}$	0.022	mgP/mgC
Π_{PO_4}	0.009	mgP/liter	$\beta_{N/C}$	0.205	mgN/mgC
Π_N	0.075	mgN/liter	$\beta_{C/\mathrm{chl.A}}$	40	mgC/mg.chl.A
γ_f	0.15	1/day	$\beta_{O_2/C}$	2.67	mg O_2/mgC
μ_f	0.4	1/day	$\beta_{O_2/N1}$	3.4	mg O_2/mgN
w_{gf}	0.4 (0.2)[1]	m/day	$\beta_{O_2/N2}$	1.1	mg O_2/mgN
K_{BOD}	0.36	1/day	β_{P/O_2}	0.008	mgP/mg O_2
η	0.9 (0.95)[1]	—	β_{N/O_2}	0.08	mgN/mg O_2
ϕ	0.6	—	β_{P/O_2}^{ant}	0.0165	mgP/mg O_2
Π_{O_2}	1.0	mg O_2/liter	β_{N/O_2}^{ant}	0.28	mgN/mg O_2
ν_{N1}	0.24	1/day	ζ_e	22.0	liter/ m^2h
ν_{N2}	8.0	1/day	ζ_i	11.5	liter/ m^2h
υ_{DN}	0.0 (1.4)[1]	1/day	$Q_{PO_4}^{sed}$	0.	mgP/ m^3h
a	57. (29.)[1]	mg O_2/ m^2h	$Q_{NH_4}^{sed}$	0.	mgN/ m^3h
b	0.66	—	$\beta_{m^3/\mathrm{liter}}$	0.001	m^3/liter

Comment: 1. The values used in the two-dimensional version of the model.

In the numerical experiments performed with the two-dimensional version of the model, the Ciénaga-de-Tesca Lagoon was approximated by a computational grid with 49×111 nodes and steps of 100 m. The time step was equal to 10 sec. The location of the main sources of pollution (Fig. 2.7) and the parameters of their wastes (Table B.3) were specified on the basis of the data taken from [133]. The threshold coefficient of the horizontal turbulent diffusion of admixtures was set equal to 0.5 m^2/sec.

Table 5.3. Harmonic Constants of the Main Components of Tides in the Cartagena Harbor

Wave components	Amplitude, cm	Phase, degrees
M_2	7.7	137
S_2	1.6	047
N_2	2.4	112
K_1	9.7	240
O_1	5.9	240

The numerical calculations were performed in two versions: for the conditions of the dry and rainy seasons of the year. In the dry period of a year (January–April), the water exchange between the lagoon and the open sea is absent. Therefore, the influence of trade winds (blowing from the northeast with speeds of up to 8 m/sec) on the circulation of waters in the basin is predominant. In the rainy period of a year, the winds are weak (the daily average speed ≈ 3 m/sec) and the water exchange with the sea is realized through the strait located in the north part of the lagoon. Hence, in this case, the tidal oscillations of the level of water on the open boundary with the sea exert the decisive influence on the circulation of waters in the Ciénaga-de-Tesca Lagoon.

The numerical experiments with the model for the rainy period of the year were carried out under the following conditions: On the boundary with the sea, we set the tidal oscillations of the sea level computed on the basis of the data from [119] on the harmonic constants of the main components of tides in the Cartagena Harbor (Table 5.3). The width and depth of the strait connecting the lagoon with the sea were set equal to 100 and 1 m, respectively,. The daily cycle of the wind speed was specified on the basis of the many-year average data of observations accumulated at the "Cartagena Airport" meteorological station for October. In this case, the direction of the wind was regarded as invariable and equal to 220°.

In the dry season of the year, the strait is closed, i.e., the water exchange with the sea is absent. Thus, in the numerical calculations, we take into account the phenomenon of lowering of the level of water in the lagoon as a result of intense evaporation (about 169 mm/month) and the absence of precipitation. The numerical estimates show that, despite the absence of water exchange with the sea, the level of water in the basin dies not undergo significant variations because the decrease in the amount of water as a result of evaporation is, in fact, compensated by the supply of waste waters whose volume is equal to 69,870 m^3/day. We specify the north–northeast trade winds with a daily cycle of variations of the wind speed.

The calculations were carried out for 30 days of the model time. The numerical results show that this time period is sufficient for the variables of the model to approach a conventionally stable mode under the invariable external conditions.

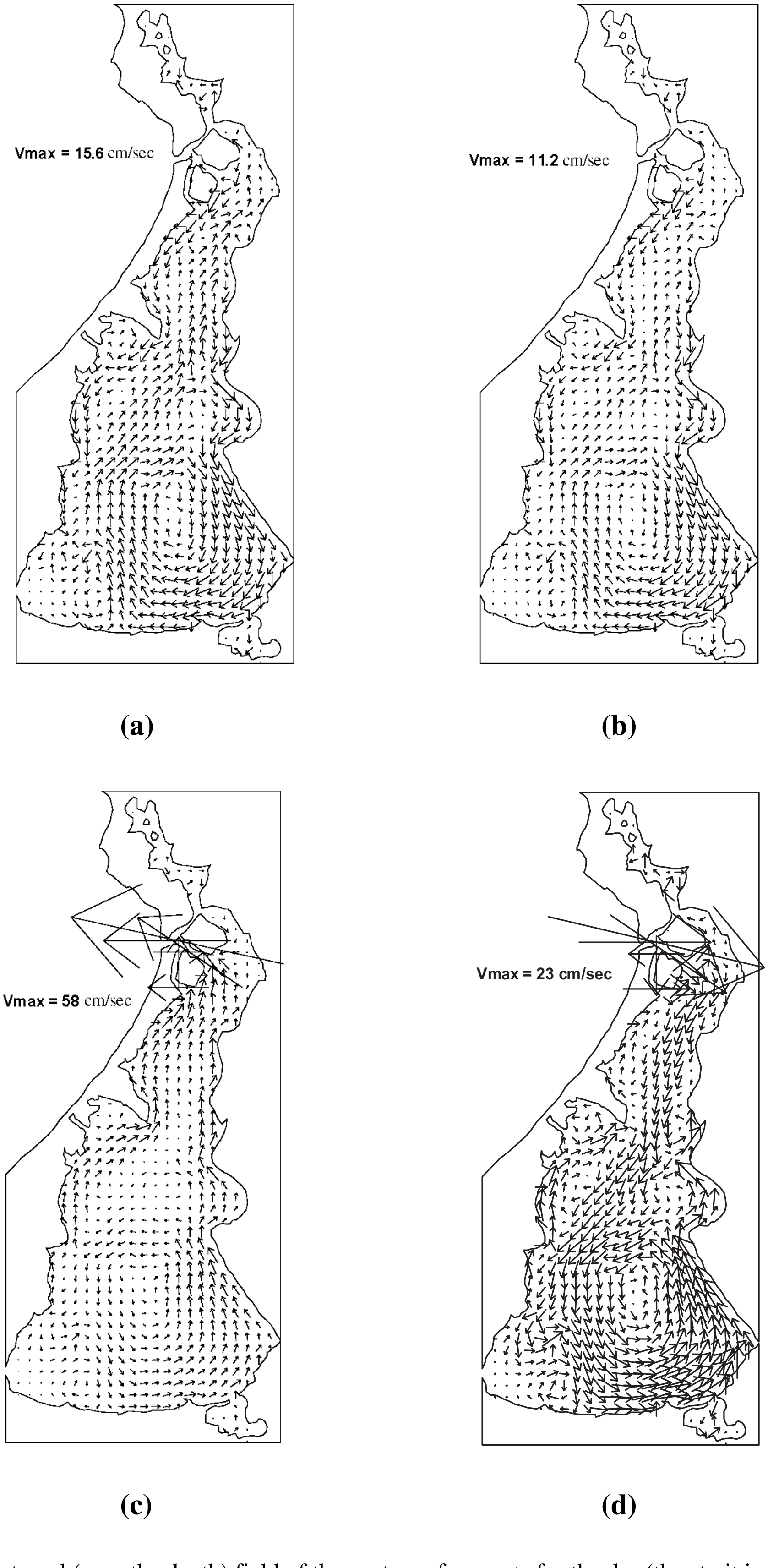


Fig. 5.13. Integral (over the depth) field of the vectors of currents for the dry (the strait is closed; (a) 0 h, (b) 12 h) and rainy (the strait is open; (c) 0 h, (d) 10 h) seasons of the year.

At the initial time, we set a uniform space distribution of the variables of the model over the area of the basin according to the data given in Table 2.2.

In Fig. 5.13, we present the integral (over the depth) fields of (barotropic) currents in the Ciénaga-de-Tesca Lagoon typical of the dry and rainy periods of the year. In the dry season, the strait is closed and the character of circulation of waters is completely determined by the daily variability of the wind speed (it is assumed that the direction of trade winds remains constant). Near the west and east coasts of the basin, we observe the formation of flows directed along the wind (in the north–south direction). At the same time, a compensating flow of the opposite direction appears in the central deeper part of the basin (Figs. 5.13a, b). The maximum velocity of currents at medium depths varies during a day from 10 to 20 cm/sec in agreement with the daily cycle of wind speed. In the south part of the water area, we detect the formation of a stationary anticyclonic gyre. At the same, ordered eddy structures do not appear in the shallow-water narrow north part of the lagoon and the field of currents is very irregular.

In Figs. 5.13c, d, we present the integral (over the depth) structure of currents typical of the rainy season and formed under the influence of tides (because the strait is open) and weak southeast winds. We readily reveal the intense water exchange through the strait in the north part of the lagoon characterized by the current velocities varying within the range 20–60 cm/sec depending on the phase of the tide.

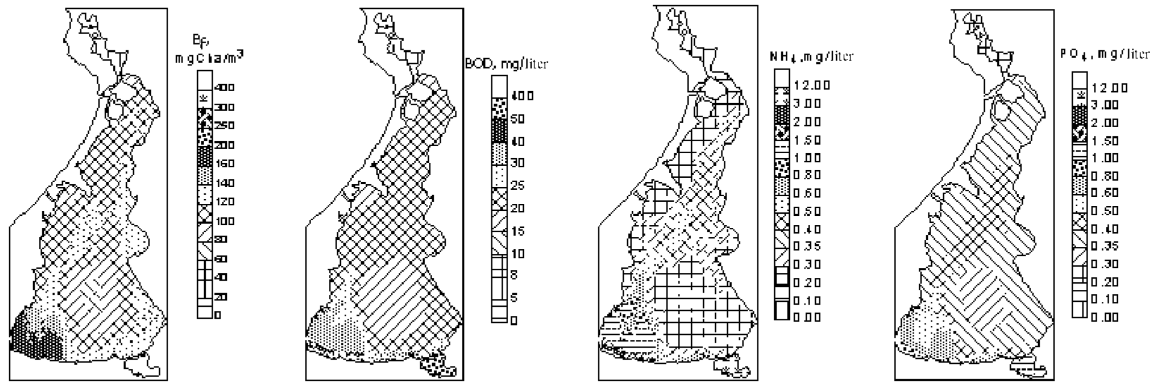
In the rainy season, the system of circulation of waters in the lagoon turns into the opposite (as compared with the dry season). In the south part of the basin, we observe the formation of a stationary cyclonic gyre whose intensity weakens in the phase of decrease in the sea level (falling tide) (Fig. 5.13c) and strengthens in the phase of elevation of the level (rising tide) (Fig. 5.13d).

The results of determination of the typical space distributions of some modeled variables of state of the Ciénaga-de-Tesca ecosystem in the dry and rainy seasons of the year are presented in Fig. 5.14 for the 30th day of model time. In the rainy season, due to the presence of more favorable conditions of illumination for photosynthesis, the production of phytoplankton and, hence, the utilization of mineral compounds of nitrogen and phosphorus by phytoplankton exceed the same parameters for the rainy season. Therefore, for the whole basin, the concentrations of inorganic biogenic substances are higher in the rainy period of the year.

In the dry season, the maximum biomasses of phytoplankton and concentrations of inorganic compounds of biogenic elements and inert organic matter are observed in the southwest part of the water area. The space distributions of the mineral compounds of nitrogen and phosphorus are characterized by the presence of a tongue of elevated concentrations elongated from the southwest part of the water area toward its northeast part and corresponding to the compensating current directed against the wind (Fig. 5.13).

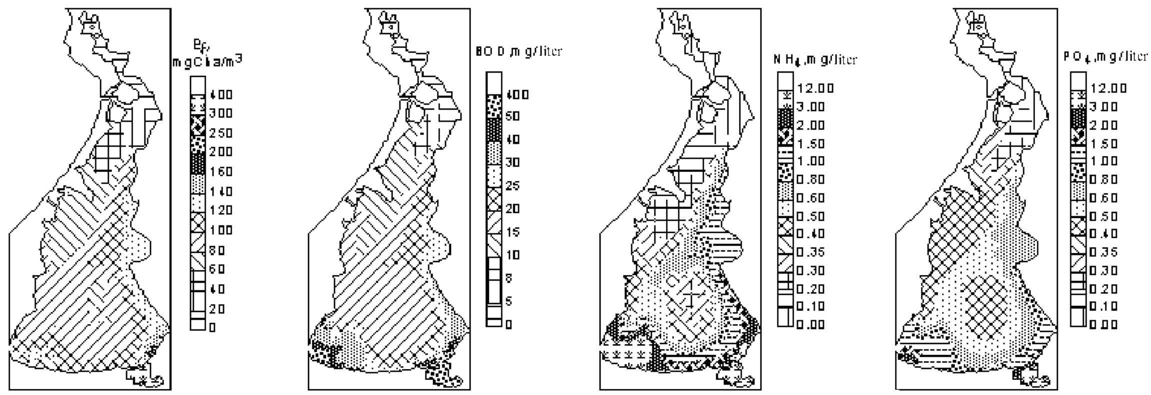
In the rainy season, the system of currents and the distribution of modeled characteristics of the ecosystem vary under the influence of the water exchange with the sea, changes in the predominant direction of the winds, and decrease in the wind speed. Large biomasses of phytoplankton and high concentrations of the mineral compounds of biogenic elements and inert organic matter are observed along the south and east coasts of the water basin.

I



(a) **(b)** **(c)** **(d)**

II



(a) **(b)** **(c)** **(d)**

Fig. 5.14. Space distributions of: (a) the biomass of phytoplankton, mg chl.A / m^3, (b) inert organic matter, mg O_2 / liter, (c) ammonium, mgN/liter, and (d) phosphates, mgP/liter, obtained by using the model for the contemporary conditions in the dry (I) and rainy seasons of the year.

The relatively clean waters of the sea propagate from the north along the west boundary of the Ciénaga de Tesca water area.

The results obtained with the help of the model agree with the data of observations both by the order of the obtained values of modeled variables and by the typical trends of their space and time variability [123, 162].

5.3.2. Calibration of the Model for the Ciénaga-Grande-de-Santa-Marta Firth

Since the mean depth of the Ciénaga-Grande-de-Santa-Marta Firth is equal to 1.6 m, we use the two-dimensional modification of the model to study the dynamics and quality of waters in this basin.

In the process of modeling, we studied the indicated basin without the Pajarales system of small lakes neighboring with the firth. In this case, the water and mass (inorganic nitrogen and phosphorus, organic substances, etc.) exchange between the firth and the Magdalena River through the system of channels and the Pajarales complex of lakes was found by using the hydraulic model of water balance [151] and taken into account in specifying the boundary conditions.

The calibration of the zero-dimensional version of the model of eutrophication of the firth was realized in the asymptotic mode for the annual average hydrometeorological conditions (the flux of PAR and the discharge of rivers and channels). The duration of numerical computations was equal to 100–300 h of model time. In the course of numerical experiments, we find the values of the parameters and coefficients of the model with the help of which the required daily course of modeled elements of the ecosystem is established after a certain period of time. Moreover, the values of the elements corresponding to the morning hours of a day in the established daily course must agree with the data presented in Table 2.4 because the observations were performed in this period of a day.

In finding the values of the parameters specifying the primary production of phytoplankton, we use the data of specialized *in-situ* experiments [136, 137, 149].

The contributions of river discharge and water exchange through the channels to the formation of hydrochemical conditions in the firth are described by using relation (5.1).

The dependence of the attenuation coefficient of the intensity of light with depth on the biomass of phytoplankton (Fig. 5.15b) is described by an empirical equation of the form $a = 2.8 + 0.028 B_{f,\mathrm{chl.A}}$, where $B_{f,\mathrm{chl.A}}$, mg chl.A/m^3, is the biomass of phytoplankton obtained on the basis of the analysis of the data of observations over the concentration of chlorophyll A and the transparency of waters in the central part of the firth.

In order to use the entire collection of data accumulated for the two decades of ecological monitoring and the results of specialized experiments, the zero-dimensional version of the model was calibrated both for the conditions of the 1980s, when mineral nitrogen limited the primary production of organic substances by phytoplankton, and for the conditions of the 1990s, when the indicated role was no longer played by mineral nitrogen.

The results of numerical experiments show that, in order to reflect in the model the transition of the ecosystem of the firth from the stationary state observed in the 1980s to its mean statistical state in the 1990s, it suffices to correct the values of the following three parameters: the ratio of the concentrations of organic carbon and chlorophyll A in the cells of phytoplankton (should be made three times smaller) and the specific rates of growth and natural mortality of phytoplankton (should be elevated by 20%). Moreover, it is necessary to make the fluxes of mineral compounds of biogenic elements from the bottom sediments and the absorption of oxygen by the bottom sediments several times more intense. This correction corresponds to the existing theoretical concepts concerning the transformations running in water ecosystems as the level of their trophicity increases.

It is known that the intensification of the process of eutrophication of marine ecosystems gives advantages to the development to small-size species of algae characterized by high concentrations of chlorophyll A in the cells and shorter life cycles (higher death rates).

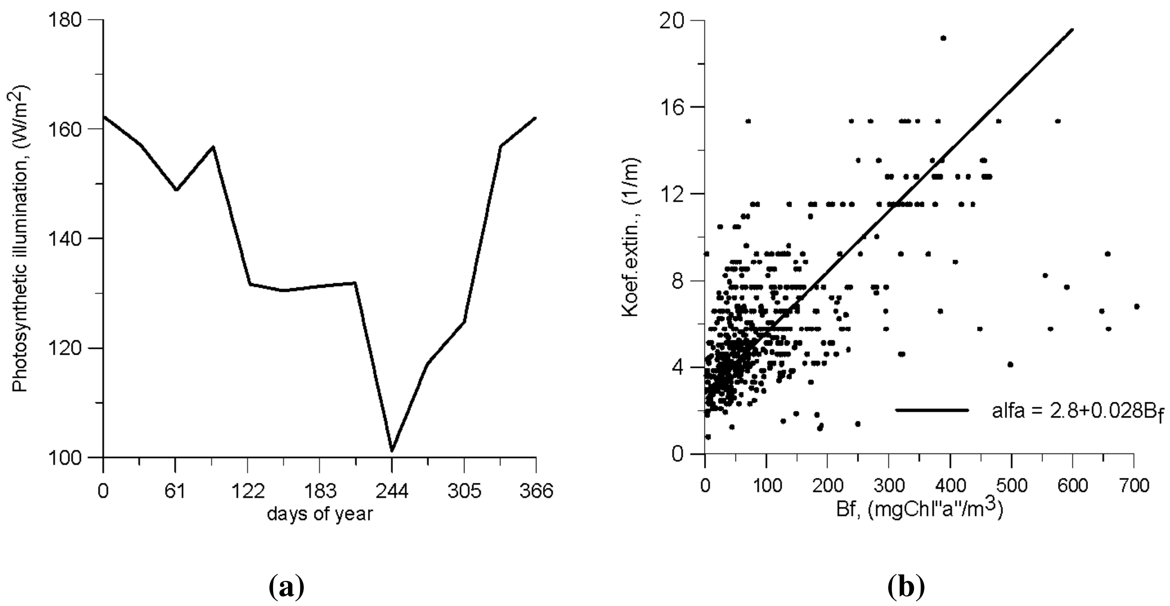


Fig. 5.15. Intraannual variability of the flow of PAR, W/m^2, (a) and the empirical dependence of the attenuation coefficient of light, 1/m, on the concentration of chlorophyll A, mgchl.A/m^3, in waters of the firth (b).

The elevation of the primary production of the ecosystem accompanying the development of eutrophication leads to the increase in the amounts of organic substances coming to the bottom sediments and the products of their decomposition coming from the bottom sediments into the bulk of water.

For some variables of the model, the dynamics of approaching the stationary state corresponding to the state of the ecosystem in the 1990s (see Tables 2.3 and 2.4) is shown in Fig 5.16.

The calibration of the point version of the model in the dynamic mode was not realized due to the absence of data on the variability of the components of water balance in the firth for the period of ecological monitoring carried out in the 1990s and the data on the relative humidity of air and cloud amount (required for the evaluation of the variability of the flow of PAR).

In passing to the two-dimensional version of the model, it is necessary to perform an additional correction of some constants of the model, since the accumulated results are affected by the morphological features of the firth and the location of the sources of pollution. In addition, unlike the point version, the two-dimensional version of the model describes the process of water exchange between the firth and the open sea.

The values of the parameters and coefficients of the model accepted after its calibration are presented in Table 5.4.

In the numerical experiments with the two-dimensional version of the model, the water area of the firth is approximated by a computational grid with 138×156 nodes and steps of 200 m. The threshold coefficient of horizontal turbulent exchange is set equal to 0.6 m^2/sec. The time steps the hydrodynamic and chemical-and-biological blocks of the model are set equal to 20 sec and 1 h, respectively.

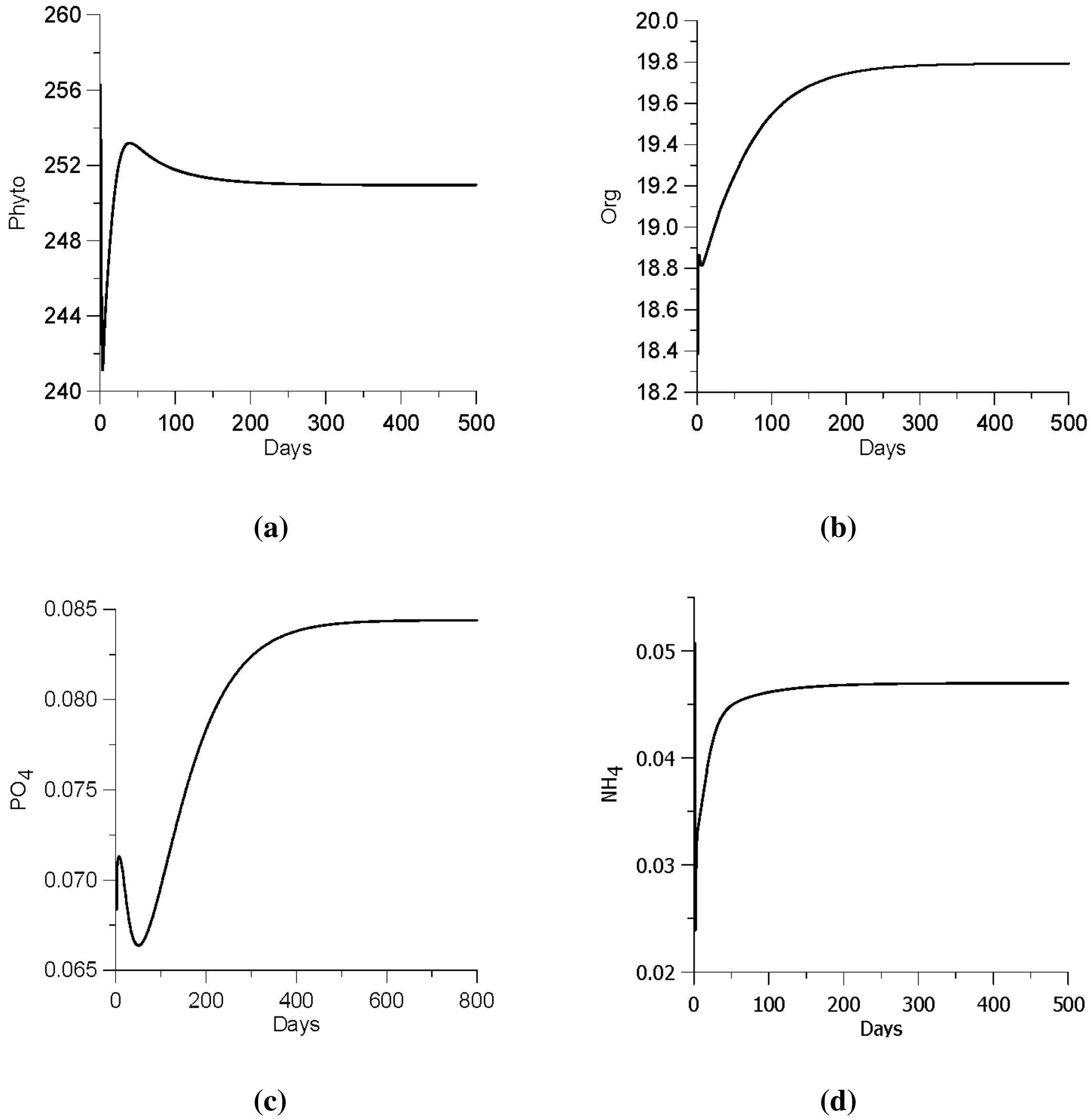


Fig. 5.16. Dynamics of attainment of the stationary state by the variables of the point version of the model under the conditions of invariable influence of the external natural and anthropogenic factors upon the ecosystem: (a) biomass of phytoplankton, mg chl.A/m^3, (b) inert organic matter, mg O_2/liter, (c) phosphates, mgP/liter, (d) ammonium, mgN/liter.

The seasonal variability of PAR (Fig. 5.15a) was determined on the basis of the many-year monthly average data on the annual course of the relative humidity of air and cloud amount in the analyzed region. On the open sea boundary, we specified the tidal oscillations of the sea level [119].

The numerical analyses according to the two-dimensional version of the model were performed for four typical months of the year: March, May, July, and October. The duration of computations was equal to 20 days. The data of numerical experiments show that the indicated time interval is sufficient for the attainment of the space distribution of the modeled variables of state of the ecosystem.

Table 5.4. Values of the Parameters of the Model of Eutrophication of Waters of the Ciénaga-Grande-de-Santa-Marta Firth Obtained as a Result of Its Calibration on the Basis of the Literature Data and the Data of Ecological Monitoring

Parameter	Value	Units	Parameter	Value	Units
V_f^{max}	10.0	1/day	$\rho_{4,d}$	0.2	—
Π_{PO_4}	0.006	mgP/liter	$\beta_{P/C}$	0.024	mgP/mgC
Π_N	0.025	mgN/liter	$\beta_{N/C}$	0.176	mgN/mgC
γ_f	0.2 (0.1)[1]	—	$\beta_{C/chl.A}$	18	mgC/mg.chl.A
μ_f	0.5 (0.4)[1]	1/day	$\beta_{O_2/C}$	2.67	mg O_2/mgC
I_{opt}	95	W/m^2	$\beta_{O_2/N1}$	3.4	mg O_2/mgN
V_b^{max}	1.5	1/day	$\beta_{O_2/N2}$	1.1	mg O_2/mgN
Π_{org}	3750	mgC/m^3	ν_{N1}	0.3	mg O_2/mgC
V_b^{max}	2500	mgC/m^3	ν_{N2}	3.0	mg O_2/mgC
Π_{O_2}	1.0	mg/liter	ϕ	0.95	—
E	0.33	—	$\beta_{m^3/liter}$	0.001	m^3/liter
V_z^{max}	0.75	1/day	a	12. (27.)[1]	mg O_2/m^2h
γ_z	0.1	1/day	b	0.66	—
μ_z	0.12 (0.07)[1]	1/day	ζ_e	22.0	liter/ m^2h
Π_z	4150	mgC/m^3	ζ_i	11.5	liter/ m^2h
$\eta_i,\ i=1,\dots,4$	0.6	—	$Q_{PO_4}^{sed}$	0.319 (0.35)[1]	mgP/ m^2h
$\rho_{1,f}$	0.5	—	$Q_{NH_4}^{sed}$	2.88 (2.67)[1]	mgN/ m^2h
$\rho_{2,b}$	0.2	—	w_g	0.1	m/day
$\rho_{3,z}$	0.1	—			

Comment: 1. The values used in the two-dimensional version of the model.

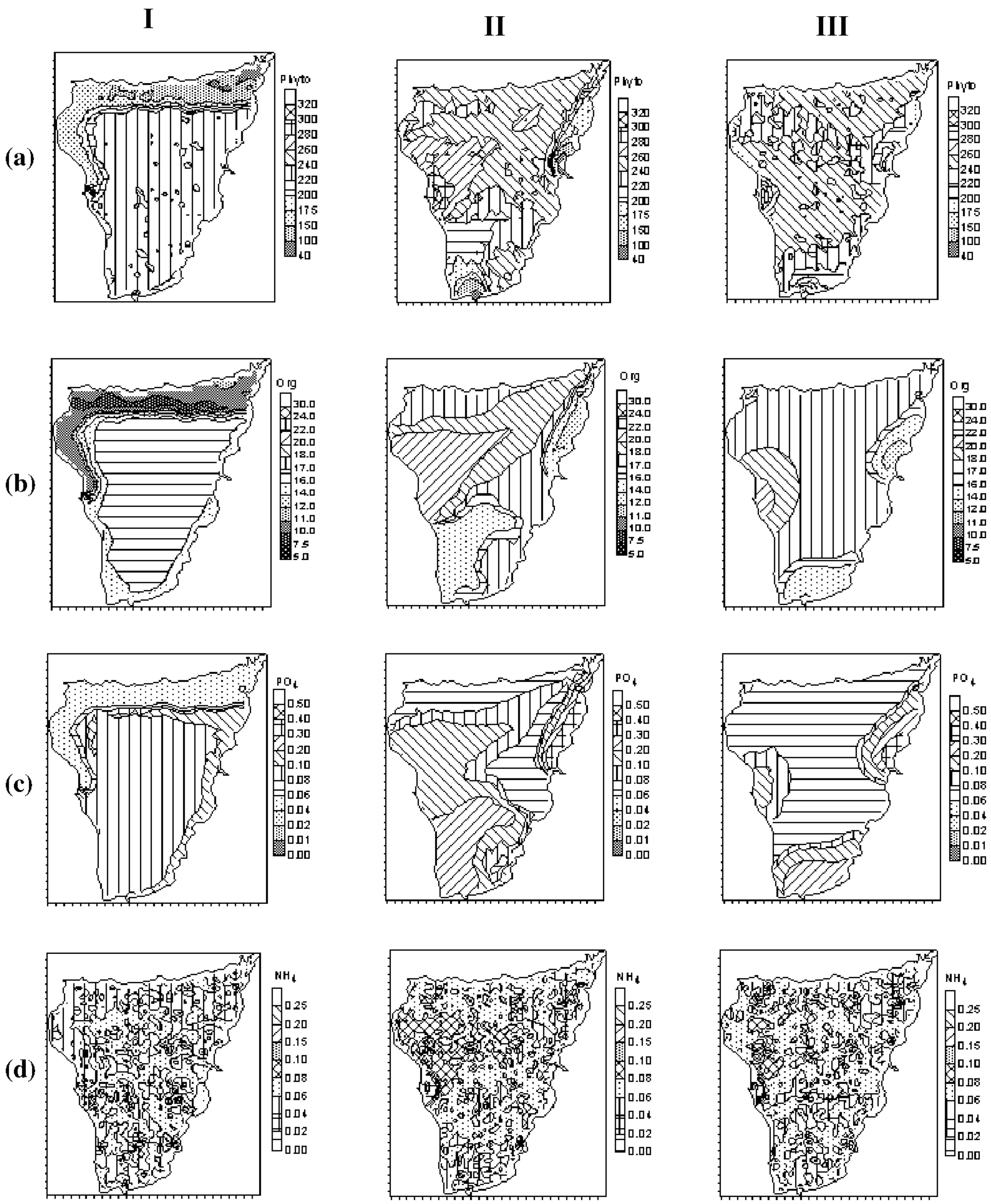


Fig. 5.17. Typical space distributions of: (a) the biomass of phytoplankton, mgchl.A/m^3, (b) the concentration of inert organic matter, mg O_2 /liter, (c) the concentration of phosphates, mgP/liter, and (d) the concentration of ammonium nitrogen, mgN/liter, obtained by using the model for March (I), May (II), and July (III).

The results of the numerical analysis of the distributions of elements of the ecosystem of the firth for the typical conditions of March, May, July, and October are presented in Figs. 5.17 and 7.23.1.

The accumulated numerical results also show that, in the dry season of the year (when the river discharge is minimum), the water exchange through channels is directed from the sea into the firth and then from the firth into the neighboring small lakes (see Table 2.5). As a result, relatively pure waters from the sea with low contents of inorganic compounds of biogenic elements and organic substances penetrate into the central part of the firth. In the dry season, the production of phytoplankton is limited by the low content of mineral nitrogen in waters of the firth because its supply by the external sources is minimum. The content of mineral phosphorus in waters of the firth, in the sources of its pollution (rivers and small lakes), and in a part of the sea neighboring with the firth significantly exceeds the values limiting photosynthesis (see Tables 2.4 and 5.4). Therefore, the seasonal variations of the concentration of phosphates do not exert any significant influence on the primary production of organic substances in the ecosystem of the firth.

In the short rainy season (May), the river discharge increases and the water exchange with the neighboring lakes is directed toward of the firth. Since the level of water in the firth in this period is higher than in the sea, the water exchange with the sea has almost no positive effect on the concentration of pollutants in the water basin due to their dilution. As a result, in view the inflow of mineral nitrogen and phosphorus with waters of the Magdalena River through the system of channels and lakes and waters of small rivers, the biogenic elements no longer limit the production of phytoplankton and it is completely determined by the illumination of the water column which, in turn, depends on the concentration of mineral and organic suspension in waters of the firth.

In July, the river discharge is close to its annual average values and the deviations of the levels of water in the lakes and firth from the sea level are minimum (Table 2.6). As a result, the level of trophicity of waters in the firth decreases as compared with the level observed in May but still exceeds the levels obtained for the dry season (March).

In October (Fig. 7.23.1), the main influence on the concentrations of mineral compounds of biogenic elements and inert organic matter in the firth is exerted by the penetration of polluted waters from the Magdalena River through the system of channels and lakes. In this period of the year, the transparency of waters in the firth is minimum and the contents of mineral and organic suspensions and organic substances are maximum.

The indicated trends of seasonal variability of the characteristics of the ecological state of waters in the Ciénaga-Grande-de-Santa-Marta Firth determined according to the results of modeling in the course of calibration of the two-dimensional version of the model agree with the data of ecological monitoring [147, 160].

As a verification of the model, one can also consider the results of the solution of the problem of self-cleaning of waters of the firth from DDT with assimilation of the data of observations [147] over its concentration in waters of the sources of pollutions (rivers and channels) in the central part of the water area of the firth obtained in November 1999. According to the data of monitoring, the concentrations of DDT were equal to $23\ \text{ng/liter}$ in waters of the Fundacion River, $79\ \text{ng/liter}$ in waters of the Aracataca River, and 2 and $6\ \text{ng/liter}$, respectively, in the Grande and Clarin Channels. In the central part of the firth, the degree of pollution was equal to $3\ \text{ng/liter}$. The rate of degradation of DDT in freshened seawater was set equal to $0.8 \cdot 10^{-7}\ \text{sec}^{-1}$ [68].

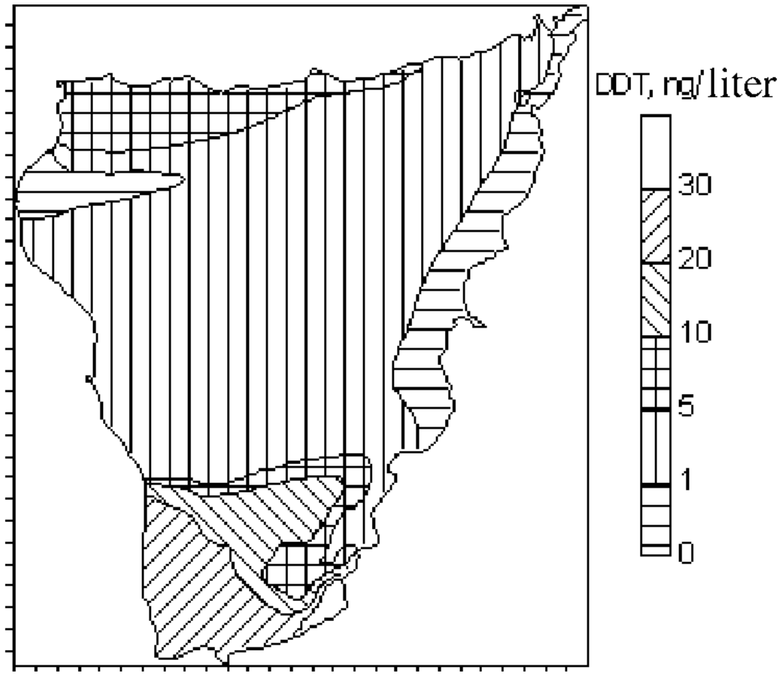


Fig. 5.18. Field of concentrations of DDT, ng/liter, in waters of the firth obtained according to the model of self-cleaning for the conditions of November 1999.

The results of the analysis of pollution of the water area of the firth (Fig. 5.18) performed according to the model of self-cleaning of waters for the rainy season are in good agreement with the data of observations carried out in the central part of the firth.

5.3.3. Calibration of the Model for the Cartagena Bay

Note that the depths observed in the Cartagena Bay can reach 26 m, the depth of the photic layer ≈ 4 m, and the depths of the straits connecting the bay with the sea are smaller than 3 m (with the exception of the narrow navigation channel). Therefore, the mathematical model used for the description of the dynamics and quality of waters in the bay should be three-dimensional.

The preliminary evaluation of the parameters of the block of eutrophication is performed on the basis of the data of literature sources on the most probable values of the specific rates of chemical and biological processes in warm eutrophic waters. By using the empirical dependences available from the literature (see Section 5.1), the parameters of the model are reduced to the *in-situ* temperature conditions (the temperature of water $\approx 30°$ for the whole year). Moreover, we performed a series of specialized *in-situ* and laboratory experiments in the course of which we determined the rates of biochemical oxidation of organic substances, regeneration of the mineral compounds of biogenic elements, and primary production of organic matter by phytoplankton in waters of the bay for the conditions of dry and rainy seasons, as well as the flux of absorption of oxygen by the bottom sediments at different points of the bay [152, 153].

As the principal criteria of the choice of constants of the model in the process of calibration, we used, on the one hand, the maximum possible correspondence between the dynamics of the processes described by the model and the data of *in-situ* observations and, on the other hand, the agreement of these constants with the estimates obtained by other researchers.

The procedure of calibration of the model of eutrophication of the bay on the basis of the data of *in-situ* observations was first performed for the one-dimensional version, i.e., in fact, for the model of annual dynamics of the vertical distribution of components of the ecosystem with regard for the external fluxes of substance and energy. In this stage, the main problem of calibration was to get the agreement between the orders of the observed values of components of the ecosystem and the values given by the model.

For the evaluation of the flow of PAR, the seasonal variability of the wind conditions, the discharge of the Dique Channel, the transparency of waters, and meteorological parameters were specified according to the data of many-year observations. As for the other tropical basins, the tidal oscillations of the sea level on the open boundary were set on the basis of the data on the principal harmonic components of tides in the Cartagena Harbor (see Table 5.3) [119].

The preliminary correlation analysis of the data of monitoring enables us to establish the contribution of mineral suspension to the attenuation of the intensity of light in waters of the bay with depth [142]:

$$\alpha_{sus} = 1.31 C_{sus}^{0.542}, \tag{5.5}$$

where C_{sus}, mg/liter, is the concentration of mineral suspension in the surface layer.

In the numerical calculations, we used the following formula:

$$\alpha = \alpha_0 + \alpha_{sus} + \alpha_f,$$

where α, 1/m, is the total attenuation coefficient of light with depth, α_0 is the extinction coefficient typical of the oceanic waters, and α_{sus} and α_f are, respectively, the coefficients reflecting the contributions of mineral suspension and phytoplankton to the attenuation of the flow of PAR. Moreover, according to [76], we have

$$\alpha_f = 0.0088 B_{f,\text{chl.A}} + 0.054 B_{f,\text{chl.A}}^2, \tag{5.6}$$

where $B_{f,\text{chl.A}}$ is the concentration of chlorophyll A in the photic layer.

The numerical experiments with the one-dimensional model were carried out in two stages. In the first stage (asymptotic calibration), the main aim of calculations was to get, under the invariable external actions (annual average conditions), a stable vertical distribution of elements of the model corresponding to the actual distribution. This aim was attained by correcting (within the allowable limits) the initial values of the parameters of the chemical-and-biological block of the model of eutrophication determined in the stage of precalibration.

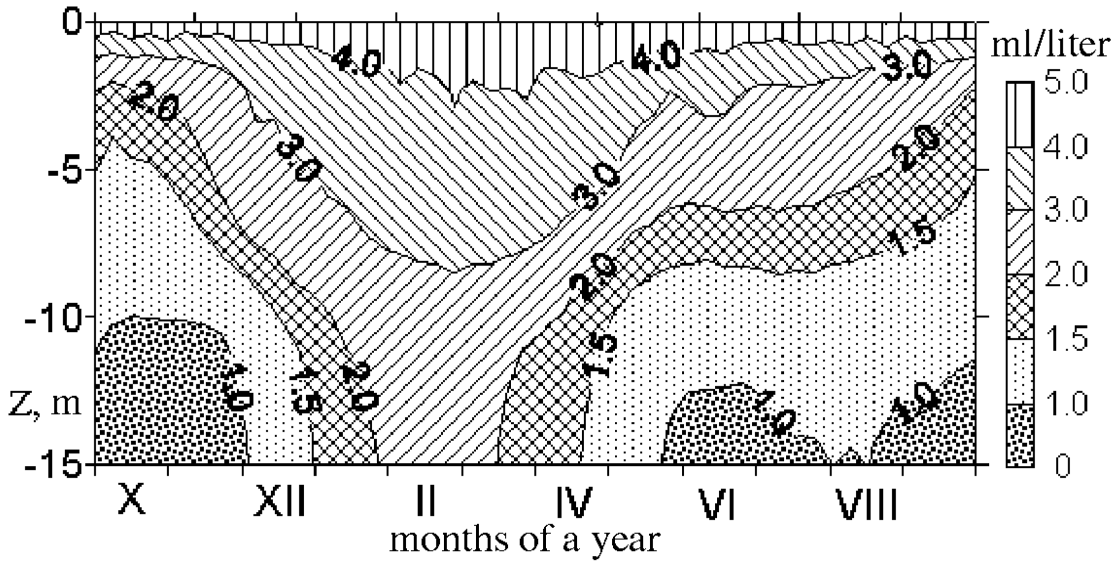


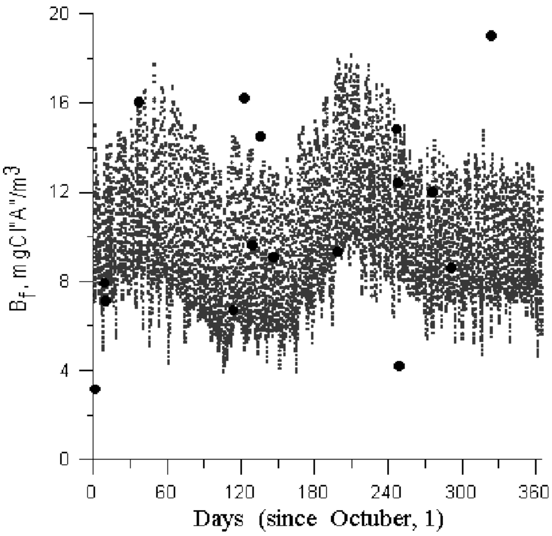
Fig. 5.19. Intraannual variability of the vertical distribution of oxygen of in waters of the Cartagena Bay, ml / liter, obtained in the process of calibration of the one-dimensional version of the model.

In the second stage (dynamic calibration), the problem was supplemented with the annual climatic course of PAR, wind velocity, discharge of the Dique Channel, and salinity of the surface layer of the bay. Thus, we performed the repeated correction of the parameters and coefficients of the model for the attainment of the maximum possible correspondence between the computed seasonal variability of modeled elements of the ecosystem in the photic layer and their actual variability determined as a result of observations. The values of constants obtained as indicated above are then used in the three-dimensional version of the model.

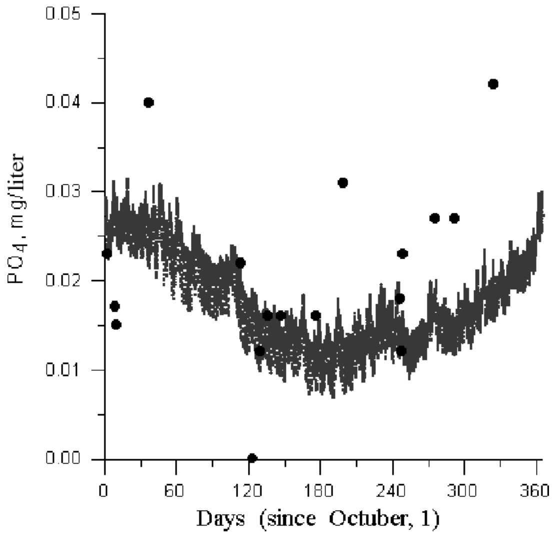
Some results of calibration of the one-dimensional version of the model are presented in Figs. 5.19 and 5.20. Despite the significant formalization of the problem, the variations of the chemical and biological elements of the ecosystem obtained in the model correspond, in general, to the data of *in-situ* observations (see Subsection 2.1.1). In the bottom layer, the maximum concentrations of dissolved oxygen correspond to the dry season, whereas the minimum concentrations correspond to the short and long rainy seasons (Fig. 5.19). Unfortunately, the absence of a single complex of observations over the internal and external factors specifying the dynamics of the components of the ecosystem in the bay does not allow us to perform a more exact calibration of the model.

In the numerical experiments with the three-dimensional model, the water area of the Cartagena Bay was approximated by a computational grid with 37×64 nodes and steps of 250 m. The time steps were equal to 12 sec in the hydrodynamic block and to 1 h in the chemical-and-biological block. The threshold value of the coefficient of horizontal turbulent diffusion was set equal to $1.0\,m^2/sec$. We used ten levels along the vertical for numerical computations.

The typical space distributions of elements of the ecosystem in the water area of the bay were computed for the dry and rainy seasons of the year.



(a)



(b)

(c)

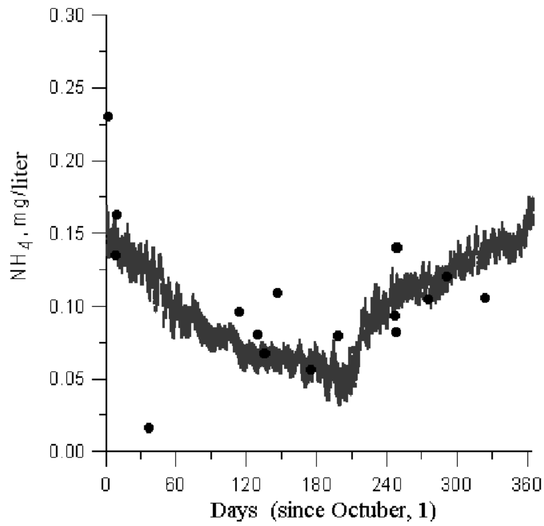


Fig. 5.20. Intraannual variability of: (a) the biomass of phytoplankton, mgchl.A/m^3, (b) ammonium nitrogen, mgN/liter, (c) phosphorus of phosphates, mgP/liter, established by using the one-dimensional model (solid line) and as a result of averaging of the data of observations carried out in the bay over the space (symbols).

As earlier, the "typical" (characteristic) space distribution of the chemical and biological characteristics of the ecosystem is defined as a distribution corresponding to the stationary state approached by the ecosystem under the action of invariable external factors (anthropogenic loads and hydrometeorological conditions) for given parameters of functioning of the ecosystem.

The determination of the distributions of chemical and biological variables of state of the ecosystem typical of different seasons of the year was carried out with an aim to refine the values of parameters and check of the three-dimensional version of the model by comparing the model fields with the data of *in-situ* observations.

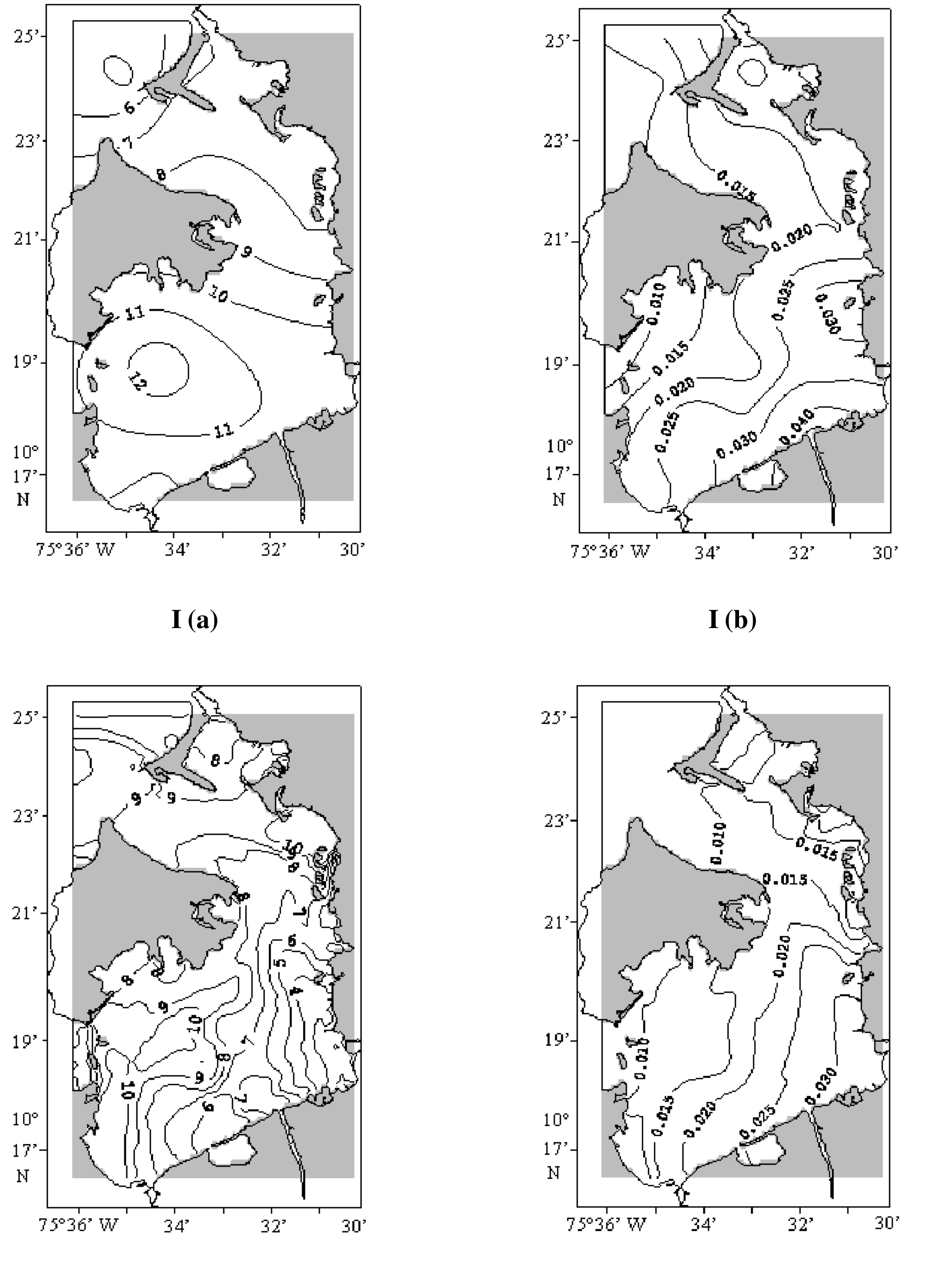


Fig. 5.21. Fields of distributions of the biomass of phytoplankton (I), mg chl.A/m^3, and the concentration of phosphates (II), mgP/m^3, in the surface layer of the Cartagena Bay in the dry season (January) obtained according to the data of observations (a) and computed by using the three-dimensional version of the model (b).

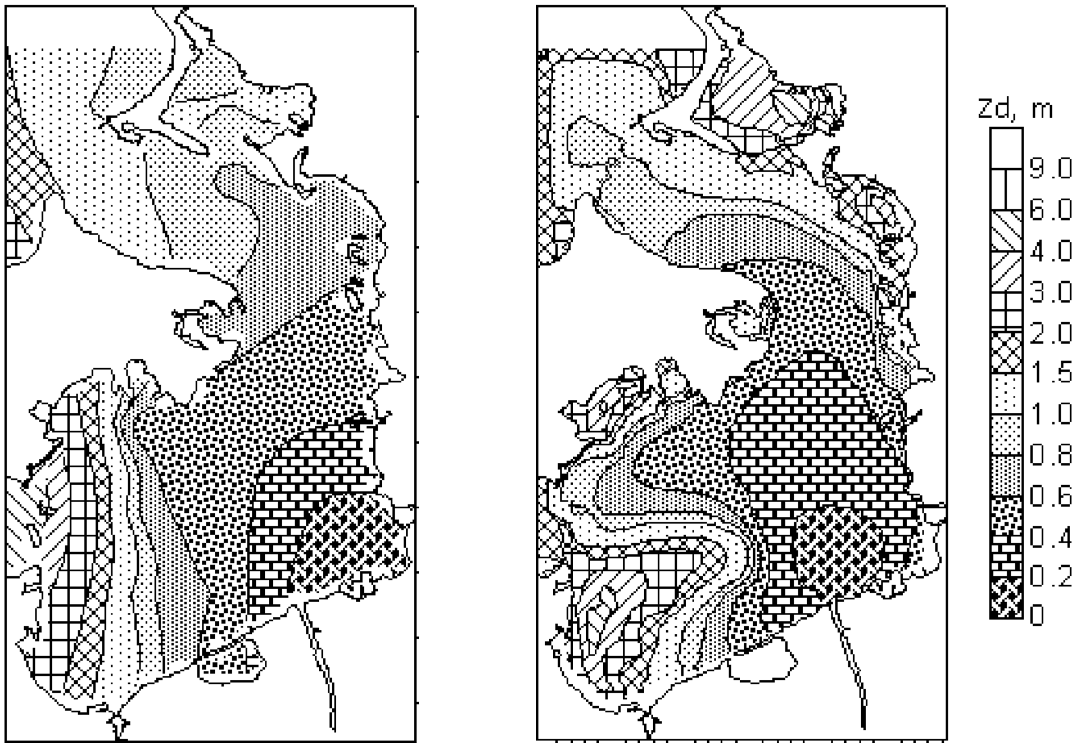
Table 5.5. Values of Constants for the Chemical-and-Biological Block of the Model of Eutrophication of the Cartagena Bay Determined as a Result of Its Calibration

Symbol	Value	Dimensionality	Symbol	Value	Dimensionality
$V_f^{\max}$	4.0	1/day	λ_f	0.4 (0.8)[1]	—
$V_b^{\max}$	2.0 (4.0)[1]	1/day	Π_{org}	1000.	mgC/m^3
Π_{PO_4}	0.01	mgP/liter	$\beta_{C/\text{chl.A}}$	40.	mgC/mg.chl.A
Π_N	0.073	mgN/liter	$\beta_{P/C}$	0.024	mgP/mgC
γ_f	0.1	1/day	$\beta_{N/C}$	0.176	mgN/mgC
μ_f	0.5	1/day	$\beta_{P/C}^{\text{ant}}$	0.034	mgP/mgC
I_{opt}	110	W/m^2	$\beta_{N/C}^{\text{ant}}$	0.51	mgN/mgC
w_{gf}	1.0	m/day	$\beta_{\text{O}_2/C}$	3.47	$\text{mg O}_2\text{/mgC}$
η_f	0.9	—	$\beta_{\text{O}_2/N1}$	3.4	$\text{mg O}_2\text{/mgN}$
δ	0.1	1/day	$\beta_{\text{O}_2/N2}$	1.1	$\text{mg O}_2\text{/mgN}$
w_{gd}	1.0	m/day	υ_{DN}	0.1	1/day
ϕ	0.2	—	υ_{phot}	0.1	1/day
Π_{O_2}	1.0	mg/liter	a	128.	$\text{mg O}_2\text{/m}^2\text{h}$
ν_{N1}	0.21	1/day	b	0.66	—
ν_{N2}	4.0	1/day	ζ_e	22.0	$\text{liter/m}^2\text{h}$
E	0.33	—	ζ_i	11.5	$\text{liter/m}^2\text{h}$

Comment: 1. The values used in the one-dimensional version of the model.

In the same stage of calibration of the model, we also determined the characteristic features of the space variations of elements of the ecosystem of the bay in the dry and rainy seasons of the year and the factors affecting these features and clarified the role of various anthropogenic sources of pollution in the process of eutrophication.

Some results of verification of the three-dimensional version of the model are presented in Figs. 5.21 and 5.22. The conditions under which we solve the problem of modeling of the transparency of waters in the Cartagena Bay are described in Section 7.6.



(a) **(b)**

Fig. 5.22. Field of transparency of waters in the Cartagena Bay for the rainy season of the year, m, plotted according to the data of observations carried out in 1996–1999 (a) and computed according to the model of self-cleaning (b).

The constants of the chemical-and-biological block of the model of eutrophication of the Cartagena Bay accepted as a result of calibration of the model on the basis of the available experimental and literature data and the data of numerical experiments performed by using the one- and three-dimensional versions of the model are presented in Table 5.5.

Conclusions

The procedures of calibration of the parameters of models of the quality of waters and verification of the results obtained by using these models are carried out on the basis of the data of ecological monitoring of the investigated water areas of the sea.

The proposed method of calibration of the blocks of eutrophication of models of the quality of waters includes the following three stages: the stage of precalibration according to the data of literature sources, the stage of direct or indirect determination of the values of the required parameters of the block in the course of special experiments, and the stage of calibration according to the data of *in-situ* observations obtained in the course of ecological monitoring.

In the first stage, it is necessary to determine the most probable values of the parameters of the model and the ranges of their variation on the basis of the analysis of the data available from the scientific literature, including highly specialized studies, and the standard values of the hydrological and hydrochemical characteristics of waters in the investigated water area. In using the model for the solution the applied ecological problems in water areas of the sea with different conditions, it is reasonable to use various handbooks generalizing the data presented in different literature sources. This problem is solved by the authors in Section 5.1. The systematized and generalized information is of great interest for a broad circle of experts using the methods of mathematical simulation for the solution of applied problems of utilization and protection of the marine resources.

The second stage of calibration is required for the adjustment of the parameters of the model to the conditions of the analyzed water area. In the course of specialized observations and experiments, it is necessary to determine the parametric characteristics of the fluxes of substances and energy between the elements of the ecosystem and their dependences on the current and standard hydrological, chemical, and biological characteristics of the water medium.

The third stage of calibration proves to be especially important since the required adequacy of the obtained model results to the data of observations is attained just in this stage. In the course of numerical experiments, the procedure of calibration of the parameters and coefficients of the chemical-and-biological block of the model of eutrophication is realized in the asymptotic and/or dynamic modes. The asymptotic method of calibration is proposed by the authors for application at tropical latitudes. The dynamic method of calibration is universal and, hence, can be used for the development of models of water ecosystems both at the tropical and middle latitudes. Moreover, this method is more representative because the data of observations are compared not only with the obtained values of modeled variables but also with the specific features of their dynamics.

First, the model is calibrated in the zero- (point) or one-dimensional (along the vertical) version. Then the obtained values of the parameters and coefficients are corrected according to the results of numerical experiments performed with the two- or three-dimensional version of the model. The zero-dimensional version is used for the precalibration of two-dimensional (without resolution along the vertical) models of eutrophication of the shallow-water basins of the sea (Ciénaga-de-Tesca Lagoon and Ciénaga-Grande-de-Santa-Marta Firth). The one-dimensional version is used for the precalibration of three-dimensional models of eutrophication for deep-water basins of the sea (Cartagena Bay and the Dnieper–Bug estuary region in the northwest part of the Black Sea), where the vertical stratification of modeled characteristics is not homogeneous.

As initial, we use the values of the specific rates of chemical and biological processes determined in the course of precalibration as the most probable values. As a rule, the parameters of the model determined as a result of special experiments are not corrected.

We propose the following scheme of correction of the parameters of the model in the third stage of calibration: In the first steps, the dynamics of the mineral compounds of nitrogen and phosphorus, inert organic matter, and dissolved oxygen is specified according to the data of observations. The parameters of equations of the dynamics of phytoplankton are varied to get the maximum possible agreement between the model curves and the observed values. Then we successively include in the system the equations for the concentrations of the mineral compounds of nitrogen and phosphorus and their parameters are corrected. After this, we add the equations for the inert organic matter and heterotrophic biotic variables of the model. Finally, we add the equation for dissolved oxygen.

As soon as all equations of the model are included in the system, the procedure of correction is realized in a sequence determined by the sensitivity of the model to the variations of some of its parameters. As a rule, the parameters of the equation of dynamics of the biomass of phytoplankton and the specific rates of biochemical oxidation and mineralization of the inert organic matter are especially significant.

The original schemes and the procedure of calibration of the block of eutrophication described in the present chapter were approved and revealed their efficiency in constructing the mathematical models of the quality of waters for the investigated water areas and basins of the sea located in different climatic zones and characterized by different morphological, hydrological, hydrochemical, and hydrobiological characteristics. Together with the methodical approaches (described in the previous chapter) to the evaluation of the parameters of the models according to the results of special *in-situ* and laboratory experiments, the proposed procedures and means of calibration form a methodology of solution of the problem of adaptation and verification of the applied models of the quality of waters for shelf sea ecosystems.

6. INFORMATION SUPPORT FOR WATER QUALITY MODELING

According to the classical definition [3], ecological monitoring is understood as a system of observations, evaluation, and prediction of the state of the environment that enables one to detect the changes in the state of the biosphere under the influence of human activity against the natural background. The developers of the concept of ecological monitoring indicated that it is based on the following two foundations: (i) a system of observations of ecological parameters and the systems analysis of their variability; (ii) a system of mathematical models on the basis of which one performs a mathematical analysis and obtains diagnostic and prognostic characteristics, which serve as a basis for making administrative decisions concerning the control of the ecological situation [79].

Being an integral part of ecological monitoring, mathematical modeling imposes special requirements on its organization [101]. To characterize the ecological state of marine environment, it suffices to set up a system of observations of some of its ecological characteristics, whereas the construction, calibration, and verification of mathematical models require the determination not only of the variability of the most important components of the ecosystem and factors affecting the system but also of the rates of all the most important processes that connect these components, realizing the circulation of substance and energy in the ecosystem. However, the problem of the determination of these rates on the basis of data of field observations is very difficult and often even essentially insolvable. For this reason, laboratory modeling of processes is widely used for the determination of these rates. Therefore, ecological monitoring must include not only standard full-scale observations of the concentration (biomass) of elements of the ecosystem but also special full-scale and laboratory experiments aimed at the determination of the flows of substance between these elements and their variability depending on the affecting factors of the environment.

6.1. Requirements for the Organization of Ecological Monitoring of Marine Environment from the Viewpoint of Mathematical Modeling

Observations of physical, chemical, and biological parameters of marine environment carried out within the framework of ecological monitoring must be complex and simultaneous. Only under these conditions can one reveal the cause-effect relationships between the characteristics of the ecosystem. For example, it is not reasonable to determine the primary phytoplankton production without observation of its main factors (the concentration of biogenic elements and the illuminance of a water column).

The ecological monitoring of marine water areas must include investigations of both time and space variabilities of the parameters of the state of marine environment. The main method for the investigation of the space variability of ecological parameters is an oceanographic survey, which must be conducted as fast as possible. The last requirement imposes restrictions on the number of measured parameters. The characteristics of the ecosystem whose determination is laborious and time-consuming are measured at a rare network of stations. For chemical and biological parameters in the case of operation in a near-shore region of the sea under field conditions, one usually performs only sampling and sample conservation with subsequent treatment under laboratory conditions.

Oceanographic stations must be located so as to reflect the typical features of the space distribution of measured characteristics. As a rule, oceanologic stations are located near known or potential sources of pollution at a certain distance determined in each individual case by the power of a source and the intensity of dilution. Some stations (called background stations) must be located at a distance from all sources of pollution such that the influence of these sources on the measured characteristics is negligible.

The number of depths of observation (sampling) at each oceanographic station is determined by the inhomogeneity of the vertical distribution of measured characteristics. In the case of a homogeneous vertical structure of waters (the absence of a pycnocline), sampling only in the surface and near-bottom layers is admitted as a necessary minimum. If, however, a pycnocline is present, then, according to oceanologic standards, the minimum number of depths increases to four (the surface layer, the upper boundary of the pycnocline, the lower boundary of the pycnocline, and the near-bottom layer). To identify the depth of location of a pycnocline, one should use oceanographic probes.

The total duration of ecological monitoring of coastal marine water areas must be correlated with its objectives and the time scales of the investigated phenomena. The duration of monitoring must at least correspond to the time cycle of the investigated phenomenon. For example, if a phenomenon is regular and seasonal, then its description requires the investigation of the annual behavior of its characteristics and factors that determine this phenomenon. If a phenomenon is seasonal but not regular, i.e., if it is observed not every year, then the duration of monitoring increases to several years. In most cases, the minimum duration of ecological monitoring is equal to one year because the one-year cyclicity in the variability of characteristics of an ecosystem is observed at both temperate and tropical latitudes.

Due to considerable consumption of material and human resources, oceanographic surveying is carried out, as a rule, once a season; in rare cases, it is carried out twice a month. Therefore, for the investigation of the time variability of characteristics of the state of marine environment, it makes sense to complement oceanographic surveying with one or several benchmark stations on which full-scale observations are performed with minimally possible time discreteness and maximum depth resolution. At the same stations, one performs all special full-scale experiments aimed at the determination of the rates of chemical and biological processes.

The realization of a mathematical model as one of the main aims of ecological monitoring imposes its requirements on the complex of observations performed within its framework. To simplify the presentation, we consider hydrometeorological, hydrochemical, and hydrobiological components of the complex of observations separately.

6.1.1. Hydrometeorological Monitoring

As is known, the hydrochemical mode, the dynamics of biotic components of the ecosystem, and the quality of its waters are formed under the defining influence of hydrometeorological factors. Therefore, a complex of observations of the variability of meteorological and hydrophysical characteristics of biogeocenoses is an integral part of the ecological monitoring of seawater quality. The most important of them are the following:

(i) the morphometric characteristic of the water area (bathymetric map);

(ii) the wind mode of the water area, the annual behavior of the velocity and direction of wind, temperature and relative air humidity, precipitation and evaporation, and the illuminance of the water surface;

(iii) the discharge of rivers and other water sources that flow into the investigated water area;

(iv) the characteristic of water exchange via straits connecting the water area with an open sea based on data of observations;

(v) the characteristic of tidal and wind-surge oscillations of the sea level at several near-shore places of the water area and at its open sea boundaries;

(vi) the space–time variability of the thermohaline stratification of waters in the investigated water area and at its open sea boundaries;

(vii) the characteristic of the three-dimensional structure of the current field based on the data of observations under known hydrometeorological conditions;

(viii) the water clarity and its dependence on the content of the mineral and organic suspension.

6.1.2. Hydrochemical Monitoring

It is recommended that a complex of hydrochemical observations aimed at the control of water quality according to the level of trophity and saprobity include, at least, the following characteristics:

(i) mineral compounds of nitrogen (ammonium, nitrites, and nitrates), phosphorus (phosphates), and silicon (silicates);

(ii) organic carbon, nitrogen, and phosphorus with separated suspended and dissolved components;

(iii) the content of dissolved oxygen;

(iv) estimates for the concentration of organic matter based on the data of oxygen consumption in the course of its oxidation: BOD_5, BOD, and the permanganate and bichromate oxidizability in filtered and unfiltered samples.

Among the hydrochemical characteristics listed above, those related to the content of organic matter in water are the most problematic. To obtain a balance in the circulation of substances in marine ecosystems, it is necessary to determine the concentration of inert organic matter, which can be in water in two fractions: dissolved and suspended (detritus). According to oceanographic standards, membrane filters with pores 0.45 μm in size are used for their separation,. In addition, in the description of the dynamics of water ecosystems, it is important to distinguish between the readily oxidizable (labile) and the relatively stable (hard-to-reach) components of detritus. Unfortunately, at present, there is no standard economical method for the direct analytic determination of these characteristics. For this reason, one has to evaluate them by using indirect hydrochemical and hydrobiological characteristics (BOD_5, BOD, permanganate and bichromate oxidizability, and organic carbon, nitrogen, and phosphorus) determined in filtered and unfiltered samples.

Despite the fact that BOD_5 is chosen as a standard hydrochemical characteristic of water quality, it does not have any real equivalent. On the contrary, the value of BOD called total in the domestic literature and carbon in the Western literature characterizes the total content of organic compounds in water capable of biochemical oxidation. Though this value is proportional to the concentration of labile inert organic matter in water, it is not equivalent to the latter because it depends on the metabolic activity not only of bacteria but also of other hydrobionts (phytoplankton and microzooplankton) in a sample.

Experimentally, the value of BOD is determined under laboratory conditions by the beginning of the nitrification reaction. For the determination of the carbon BOD, a long-term (8 to 25 days) incubation period of samples is required. The length of this time period depends on the amount of organic matter, temperature, the amount of bacteria, their metabolic activity, etc. However, BOD can be determined from BOD_5 by using the following parametric relation:

$$\mathrm{BOD} = \mathrm{BOD}_5(1. - \exp(-5K_{\mathrm{BOD}}))^{-1},$$

where K_{BOD} is the specific rate of biochemical oxidation of organic matter, day^{-1}, determined in the BOD experiment or calculated on the basis of the empirical dependence (see Sec. 5.1).

The permanganate and bichromate oxidizabilities characterize, respectively, the amount of readily oxidizable organic matter and the total amount of organic matter on the basis of chemical oxygen consumption.

Since, in the general case, the rates of regeneration of mineral compounds of nitrogen and phosphorus in the process of biochemical oxidation of organic matter can be different, the stoichiometric relations for the inert organic matter in the transition stage of decomposition are violated. Therefore, the complex of observations, in addition to BOD and oxidizability, includes the examination of organic compounds of nitrogen, phosphorus, and carbon with their separation into suspended and dissolved fractions. For the reduction of estimates for the concentration of organic matter obtained by different methods to unique carbon measurement units, one uses scaling stoichiometric coefficients [3, 15, 118, 128].

Exchange processes in the "water–bottom sediments" system essentially affect the hydrochemical mode of eutrophied shallow partially bounded shelf zones of the sea (gulfs, bays, and firths). Therefore, the determination of the flow of absorption of oxygen by bottom sediments and the intensity of exchange of biogenic substances in the "water–bottom sediments" system, depending on the content of oxygen in the near-bottom layer, is one of the most important problems in hydrochemical monitoring of such water areas.

One can point out two alternative approaches to the solution of this problem. The first approach consists of the experimental determination of the amount of oxygen absorbed by sediments for a fixed time interval (BOD of bottom sediments) and the direct measurement of the flows of mineral compounds of phosphorus and nitrogen in the "water–bottom sediments" system under aerobic and anaerobic conditions for different points of the investigated water area [29]. Using, as an example, the determination of BOD, one can describe the general scheme of an experiment as follows: The original concentration of dissolved oxygen and its value at the time of incubation are determined in an isolated volume of water that is in contact with bottom sediments. In parallel, the BOD of water without ground is determined under the same conditions. Subtracting the value of BOD of water from the total value of BOD, we obtain the biological absorption of oxygen by bottom sediments. It is expressed in mg of O_2 absorbed for the incubation time by a unit of volume, or by a unit of mass, or by the amount of absorbed oxygen divided by the area of the surface of contact of water with bottom sediments. Experiments can be carried out under different conditions by different methods:

— under natural conditions, by isolating a section of the bottom by special containers [116];

— under laboratory conditions, in running and stagnant isolated aquariums of various structures containing bottom sediments with known surface area [29].

On the basis of these experiments, one can evaluate the rate of biochemical absorption of oxygen by bottom sediments and the variability of the intensity of flows of mineral compounds of phosphorus and nitrogen in the "water–bottom sediments" system depending on the oxygen conditions in the near-bottom layer.

In the investigation of the exchange of biogenic substances in the "water–bottom sediments system," aerobic conditions are maintained by artificial aeration of water, and anaerobic conditions are maintained by periodical blowing of nitrogen through the water.

According to the second approach, one investigates in detail the chemical composition of near-bottom water, pore solutions, and bottom sediments with undisturbed vertical structure and the functional characteristics of bacteria that take part in the decomposition of organic matter and the regeneration of mineral compounds of nitrogen and phosphorus with the purpose of mathematical modeling of processes of mass exchange in the "water–bottom sediments" system [64]. Some methodological aspects of this approach are presented in [37] and in Sec. 6.2.

The disadvantage of the first approach is the local character of the obtained results both in space and in time. The disadvantage of the second approach is the large number of specialized full-scale tests required for for determination of parameters and verification of models and special requirements on a method for sampling from different layers of a column of the bottom ground.

In the general case, the complex of hydrochemical observations also includes the determination of the level of pollution of marine environment by toxic substances. Since the list of these pollutants is very large, one should preliminarily perform a test control of waste waters of potential pollution sources, seawater, and bottom sediments in the investigated water area with the purpose of the determination of the presence of one pollutant or another in it. In the system of monitoring, one includes only the pollutants whose observed or expected concentrations in the investigated water area are comparable (or greater) with the values of their maximum admissible concentrations. Furthermore, one should, first of all, control the content of the most widespread and dangerous types of pollutants, e.g., oil, polycyclic aromatic and chlorinated hydrocarbons, synthetic surface-active substances, phenols, and toxic metals (mercury, lead, cadmium, zinc, copper, arsenic, iron, manganese, nickel, and chromium), in seawater and bottom sediments.

Toxic metals in seawater can be in three main forms: in the ionic form, in organic complexes, and adsorbed onto the surface of suspended particles and bottom sediments. The most toxic are the ionic and adsorbed forms. The dissolved and adsorbed forms of metals in water are in dynamical equilibrium, which is described by the sorption isotherm. The adsorbed forms, together with suspended particles, are removed from water in the course of sedimentation and are accumulated in bottom sediments. Under certain conditions, due to the processes of desorption and diffusion, toxic metals can leave bottom sediments and return to water again, which leads to the repeated pollution of water by these toxic substances. Therefore, in the process of ecological monitoring of marine water areas, it is necessary not only to measure the concentration of a toxic substance but also to separate its suspended and dissolved forms.

In view of the ability of bottom silts to accumulate heavy metals and other toxic substances, it is recommended to include the analysis of the content of toxic substances in bottom grounds at different points of the investigated water area into the complex of hydrochemical observations. This information, first, enables one to more precisely determine the location of the main sources of pollution of water with toxic substances and, second, can be used for the prediction of the level of repeated pollution of water.

As mentioned above, the system of ecological monitoring, in addition to field observations of elements of the ecosystem (characteristics of water quality), must also include special experiments aimed at the determination of the rates of processes (flows of substances) that connect these elements. The determination of the rates of main biochemical processes considered in the eutrophication block of a water-quality model is performed, in the classical version, in experiments in closed (bottles) and open (aquariums and mesocosms) BOD-systems. The main aim of these experiments is the observation of the kinetics of the process of decomposition of organic matter and regeneration of mineral compounds of biogenic elements in seawater samples. The experiment is based on the standard scheme of determination of BOD [108] and is described in detail in [81]. However, in addition to the determination of the content of dissolved oxygen for different times of exposure of a sample, the complex of observations of the dynamics of components of a BOD-system includes, at least, the determination of the concentrations of the following substances:

— easily oxidizable organic matters according to the permanganate oxidizability;

— mineral and organic phosphorus;

— mineral (in three forms) and organic nitrogen;

— total biomass of bacteria and, in particular, heterotrophic bacteria.

Sampling for the investigation of the destruction of organic matter is performed at different points of the water area that differ in the level of pollution of waters and physicochemical conditions (temperature, salinity, and pH). The pollution level is roughly determined by permanganate oxidizability. Depending on the aims of the experiment, samples can be filtrated as follows:

— through membrane filters with pores 4–6 μm in size for the separation of zooplankton and phytoplankton;

— through filters with pores 15–20 μm in size for the filtration of microzooplankton;

— through plankton gas with pores 60–200 μm in size for the filtration of mesozooplankton and large microzooplankton.

In using the light-and-dark-bottle method, samples are aerated and placed in a thermostat. The exposure of samples is performed in the dark at a temperature either of 20°C or close to the temperature observed under natural conditions in the process of sampling. In the first two hours of incubation, the purely chemical consumption of oxygen can take place in bottles. For this reason, it is assumed that the biochemical consumption begins two to three hours after the beginning of testing. The initial concentrations of chemical substances (zero-day concentrations) should not be determined prior to this time. For the computation of kinetic characteristics of biochemical processes and the investigation of dynamics of hydrochemical characteristics, it is recommended to perform the analysis of samples every day in the first 10 days of the BOD-experiment and then to increase the time interval between analyses to several days. The total time of experiment is at least 30 days.

In addition to the light-and-dark-bottle method, the dynamics of the components of a BOD-system can be investigated in open aquariums under natural illuminance conditions with and without aeration. In this case, in addition to the parameters indicated above, one investigates the dynamics of phytoplankton and, in some cases, microzooplankton (protozoa). “Full-scale modeling” in micro- and mesocosms in isolated water regions may serve as an alternative of laboratory experiments. Examples of microcosms are 200–250 liter isolating containers placed directly into the basin. They can be of either rigid type (made of organic glass) or soft type (made of a polyethylene film fastened to foam plastic floats in the upper part and to the base in the lower part). These containers can be with or without bottom in order to take into account the exchange of chemical substances with bottom sediments [116].

In the course of experiments with BOD-systems, the values of the following parameters can be determined: the specific rates of the biochemical oxidation of organic matter, the mineralization of organic compounds of nitrogen and phosphorus, and the first and second stages of nitrification. For the determination of the constants that characterize the rates of biochemical decomposition of organic matter and regeneration of mineral compounds of nitrogen and phosphorus on the basis of experimental data, it is assumed that the kinetics of this process is satisfactorily described by the equation of reaction of the first order:

$$K = (t - t')^{-1} \ln\left(\frac{C_0}{C_t}\right), \tag{6.1}$$

where C_0 is the initial concentration of organic matter in the units of biogenic element or BOD, C_t is the concentration after time t, t' is the time for which the concentration C_0 does not change (the time of adaptation of microorganisms), and K is the specific rate of biochemical oxidation or mineralization of organic matter. For the determination of the rate of biochemical oxidation of organic matter, it is recommended to use Eq. (6.1) modified for multiple times of incubation of samples:

$$K_{\text{BOD}} = t^{-1} \ln\left(\frac{\text{BOD}_t}{\text{BOD}_{2t} - \text{BOD}_t}\right), \tag{6.2}$$

where BOD_t and BOD_{2t} are the values of BOD for multiple times of incubation (e.g., at the third and the sixth days of an experiment).

To estimate the rate of regeneration of nitrites and nitrates on the basis of the data of laboratory experiments, more complicated computation methods are used, which take into account that the first and the second stages of nitrification proceed in seawater simultaneously. There are two methods for the solution of this problem. One can directly use the equations of kinetic curves [81]:

$$C_0 = C_0^{(0)} e^{-K_{01}t}, \tag{6.3}$$

$$C_1 = C_0^{(0)} \left(\frac{K_{01}}{K_{12} - K_{01}} e^{-K_{01}t} - \frac{K_{01}}{K_{01} - K_{12}} e^{-K_{12}t} \right), \tag{6.4}$$

$$C_2 = C_0^{(0)} \left(\frac{K_{01}K_{12}}{(K_{12} - K_{01})(K_{23} - K_{12})} e^{-K_{01}t} + \frac{K_{01}K_{12}}{(K_{01} - K_{12})(K_{23} - K_{12})} e^{-K_{12}t} \right.$$

$$\left. + \frac{K_{01}K_{12}}{(K_{01} - K_{23})(K_{12} - K_{23})} e^{-K_{23}t} \right), \tag{6.5}$$

$$C_3 = C_0^{(0)} \left(1 - \frac{K_{12}K_{23}}{(K_{12} - K_{01})(K_{23} - K_{12})} e^{-K_{01}t} - \frac{K_{01}K_{23}}{(K_{01} - K_{12})(K_{23} - K_{12})} e^{-K_{12}t} \right.$$

$$\left. - \frac{K_{01}K_{12}}{(K_{01} - K_{23})(K_{12} - K_{23})} e^{-K_{23}t} \right), \tag{6.6}$$

where C_0 is the concentration of initial organic nitrogen (C_{ON}), C_1 is the concentration of the first intermediate substance (ammonia nitrogen, C_{NH_4}), C_2 is the concentration of the second intermediate substance (nitrite nitrogen, C_{NO_2}), C_3 is the concentration of the final product (nitrate nitrogen, C_{NO_3}), K_{01}, K_{12}, and K_{23} are the constants of the rate of regeneration of ammonia (K_{NH_4}), nitrites (ν_{N1}) and nitrates (ν_{N2}), respectively, and $C_0^{(0)}$ is the initial constant of initial organic nitrogen.

Using the curve of discharge of the initial organic matter, we can determine the constant of the rate of regeneration of ammonia K_{01} according to relation (6.1). Then, using the known values of K_{01} and C_1 at a certain time t, we determine K_{12}, etc., from the system of equations (6.3)–(6.6).

According to the second, more convenient, method [81], one determines the constants of the rate of nitrification on the basis of the location of maximum points on the kinetic curves of intermediate substances, i.e., by using equations that relate the maxima of concentrations to rate constants:

$$K_{12} = K_{01} \frac{C_0^{(m_1)}}{C_1^{(m_1)}}, \qquad K_{23} = K_{12} \frac{C_1^{(m_2)}}{C_2^{(m_2)}}, \tag{6.7}$$

where $C_0^{(m_1)}$ is the concentration of the initial organic matter when the concentration of ammonia is maximum, $C_1^{(m_2)}$ is the concentration of ammonia when the concentration of nitrites is maximum, $C_1^{(m_1)}$ is the maximum concentration of ammonia, and $C_2^{(m_2)}$ is the maximum concentration of nitrites. One also uses an equation that relates the constant to the time of the first maximum $(t_1^{(m_1)})$, namely

$$t_1^{(m_1)} = \ln \frac{K_{12}}{K_{01}} (K_{12} - K_{01})^{-1}. \tag{6.8}$$

This time corresponds to the maximum concentration of the first intermediate product (NH_4^+), namely

$$C_1^{(m_1)} = C_0^{(0)} \left(\frac{K_{12}}{K_{01}} \right)^{\frac{K_{12}}{K_{01} - K_{12}}}, \tag{6.9}$$

or, in dimensionless variables,

$$\tau^{m_1} = \frac{\ln \chi_2}{\chi_2 - 1}, \qquad \eta_1^{m_1} = \chi_2 - \frac{\chi_2}{\chi_2 - 1}, \tag{6.10}$$

where

$$\tau = K_{01} t, \qquad \eta_1 = \frac{C_1^{(m_1)}}{C_0^{(0)}}, \quad \text{and} \quad \chi_2 = \frac{K_{12}}{K_{01}}.$$

If the substances involved in the reaction have initial concentrations, then one introduces the corresponding corrections and η_1 takes the form

$$\eta_1^{m_1} = \frac{1 - a + \gamma a(\chi_2 - 1)}{\chi_2 - 1} a^{-1/(1-\chi_2)},$$

where

$$a = \frac{1}{(\chi_2 - 1)\chi_2(\gamma - 1)}.$$

The graphic solution of Eqs. (6.10) and (6.11) for different values of χ_2 and γ is given in [81]. Using the values of $C_1^{(m_1)}$, $t_1^{(m_1)}$, $C_2^{(m_2)}$, and $C_1^{(0)}$ determined from the experimental kinetic curves and the value of $C_0^{(0)}$ determined from experimental data as initial conditions, for given $\eta_1^{m_1}$ and γ, one determines χ_2 from the nomogram, and then, for known $t_1^{(m_1)}$ and χ_2, one determines K_{01} and K_{12} from Eq. (6.8). The rate of regeneration of nitrates K_{23} is calculated according to Eq. (6.7).

The contribution of nitrification processes to the absorption of dissolved oxygen can be evaluated by measuring the nitrogen BOD_N defined as the difference between the consumptions of oxygen detected in water samples in the presence and in the absence of an inhibitor of the process of nitrification (allyl thiourea (thiourea and ethylene thiourea) with concentration 0.5–1.0 mg/liter). However, it should be noted that, for high concentrations of ammonium nitrogen, inhibitors of nitrification with admissible concentrations are ineffective.

6.1.3. Hydrobiological Monitoring

Hydrobiological monitoring aimed at the formal mathematical description of a marine ecosystem is performed in several stages. The first stage consists of systematic full-scale hydrobiological observations aimed at the study of specific features of the space–time variability of the biomass and the number of main biotic elements of the marine ecosystem and the investigation of trophic relations in the community of hydrobionts. The main aim of this stage is to determine the trophic structure and specific features of the dynamics of biotic elements, depending on the hydrometeorological and hydrochemical factors that define them.

In the subsequent stages, the system of monitoring includes special full-scale and laboratory experiments aimed at the determination of the intensity of processes of production, metabolism, and elimination of aggregated trophic groups of biotic elements of the ecosystem, depending on their defining factors. The aims of the most important of these experiments are the following: the determination of primary production of the autotrophic chain of the ecosystem, depending on illuminance conditions, provision with biogenic elements, and water temperature, and the determination of the production and rate of metabolism of bacteria, depending on habitat conditions. The importance of these processes is explained by the fact that they connect the biotic and abiotic components of the ecosystem.

Methodological aspects of the determination of quantitative and production characteristics of the main biotic elements of the marine ecosystem are described in detail in special hydrobiological literature (see, e.g., [63, 88]). A more complicated methodological problem is the experimental determination of functional parameters of biotic elements that determine the specific rates of their production, metabolism, and elimination. It is obvious that the direct experimental determination of the entire complex of these parameters within the framework of the solution of applied problems of marine nature management is unreal, first of all, from the financial viewpoint. For this reason, for the determination of a series of parameters one uses empirical dependences and semiempirical computational schemes established in special scientific investigations that connect the required parameters with easily determined morphological characteristics of hydrobionts and factors of the environment.

Consider some methodological aspects of the estimation of the parameters of the balance equations that describe the dynamics of biotic elements of the marine ecosystem.

Since phytoplankton is a key (and often unique) biotic variable considered in water-quality models, special attention is given to the identification of the parameters of its balance equation. As follows from the results of Chap. 4, the main parameters of the process of primary production of organic matter by phytoplankton are the rate of photosynthesis maximum possible under optimal conditions $V_f^{\max}$, the illumination intensity optimal for photosynthesis I_{opt}, and the semisaturation constant Π_i^{bg} that characterize the restrictive role of biogenic elements in the process of photosynthesis.

The determination of $V_f^{\max}$ and Π_i^{bg} for a certain biogenic element under conditions optimal for photosynthesis can be carried out on the basis of data of laboratory experiments or full-scale observations of the concentration of this biogenic element in water and the intensity of the process of photosynthesis. In this case, one uses the Michaelis–Menten equation in the linear form [10], namely,

$$C_i = V_f^{\max}\left(\frac{C_i}{V_f}\right) - \Pi_i^{bg}, \tag{6.11}$$

where C_i is the concentration of the ith biogenic element in the medium, V_f is the actual specific rate of consumption of the element under these feeding conditions, $V_f^{\max}$ is the maximum possible rate of consumption of the element under optimal conditions, and Π_i^{bg} is the Michaelis–Menten constant, i.e., the concentration of the biogenic element for which $V_f = V_f^{\max}/2$.

Equation (6.11) can be solved graphically. If we plot the concentration of a biogenic element C_i on the OX-axis and the ratio C_i/V_f on the OY-axis, then the intersection of the straight line with the abscissa axis corresponds to the value Π_i and the slope of this line is equal to $1/V_f^{\max}$.

In the case of laboratory determination of the constants of semisaturation of demands of phytoplankton for mineral compounds of nitrogen and phosphorus in the process of photosynthesis, it is necessary to eliminate their joint restriction of the process of primary production, i.e., to guarantee conditions under which only one biogenic element is restrictive. This can be realized by introducing supplementary feeding (e.g., refined salts KNO_3, KH_2PO_4, etc.) into the experimental vessel [12].

The rates of reproduction, die-off, and eating away of algae can be evaluated on the basis of the data of laboratory experiments from information on the relationship between the number of living and dead cells in a certain isolated volume of water at the beginning and at the end of testing. The methodological and theoretical foundations of this experiment are presented in [114]. Prior to the formulation of the main computational relations of this method, we introduce the following notation: x_0 is the initial number of living cells of phytoplankton, x_1 is the final number of living cells, y_0 is the initial number of dead cells of phytoplankton, y_1 is the final number of dead cells, $z_1 = x_1 + y_1$ is the total number of living and dead cells at the end of experiment, t is the duration of the experiment measured in days, V_f is the specific rate of fission or reproduction of algae, and μ_f is the specific rate of natural mortality of algae.

In the accepted notation, according to [114] we have

$$\mu_f = \frac{1}{t} \ln \frac{x_1}{x_0} \left(\frac{z_1 - x_1}{x_1 - x_0} \right) \quad \text{or} \quad \mu_f = \frac{1}{t} \ln \frac{x_1}{x_0} \left(\frac{y_1}{x_1 - x_0} \right), \tag{6.12}$$

and for the computation of the rate of reproduction of algae, we get

$$V_f = \frac{1}{t} \ln \frac{x_1}{x_0} \left(1 + \frac{z_1 - x_1}{x_1 - x_0} \right) \quad \text{or} \quad V_f = \frac{1}{t} \ln \frac{x_1}{x_0} \left(1 + \frac{y_1}{x_1 - x_0} \right). \tag{6.13}$$

Relations (6.12) and (6.13) are true if organisms of zooplankton that consume algae are absent in the sample. Otherwise, it is necessary to take into account eating away of algae by zooplankton, whose specific rate can be evaluated by using the formula

$$V_z = \frac{1}{t} \left[\ln \left\{ 1 + \frac{V_f}{V_f^0} \right\} \left(\exp(V_f^0 t) - 1 \right) \right] + \ln x_0 - \ln z_1, \tag{6.14}$$

where $V_f^0 = V_f - \mu_f$ is the resulting rate of fission of algae in a culture with regard for their reproduction and natural mortality. In this case, the expression for the computation of the ration of zooplankton (the total amount of living and dead food consumed for the time of experiment t) has the form

$$r_z = \frac{V_f x_0}{V_f - \mu_f - V_z} \left[\exp(\{V_f - \mu_f - V_z\} t) - 1 \right] + x_0 - z_1. \tag{6.15}$$

The relation for the computation of the effective production of algae with regard for their reproduction, die-off, and eating away by animals can be represented as follows:

$$P_f = \frac{V_f x_0}{V_f - \mu_f - V_z} \left[\exp(\{V_f - \mu_f - V_z\} t) - 1 \right]. \tag{6.16}$$

An important information component of the hydrobiological part of ecological monitoring of marine water areas is the experimental determination of the predominant volume of cells of phytoplankton and its variability within a year cycle. Using this information, one can take into account the succession and the corresponding variability of functional characteristics of phytoplankton in this model [18, 92]. In particular, on the basis of information on the characteristic volume of cells of phytoplankton, within a certain time interval, one can evaluate the rate of gravitational settling of cells w_{gf}, the maximum growth rate $V_f^{\max}$ of phytoplankton, and other characteristics (see Sec. 5.1). Note that, at present, in deducing empirical dependences for the computation of characteristics of functional activity of various groups of phytoplankton, researchers prefer not the volume of a cell but the specific area of its surface (the ratio of the area of the surface to the volume of the cell) as a more informative morphological functional characteristic [131, 132].

The optimal values of illumination intensity in eutrophic regions of the sea can be determined by the analysis of data of full-scale observations of the depth of location of the layer with maximum production of phytoplankton or by performing special laboratory experiments with variation in illumination intensity in the case of optimal provision of cells of phytoplankton with biogenic elements (see, e.g., [109]).

As a rule, in the investigation of ecosystems of eutrophied marine water areas, in addition to the production of organic matter by autotrophs, considerable attention is given to processes of biochemical oxidation of organic matter and regeneration of mineral compounds of nitrogen and phosphorus. These processes run with participation of heterotrophic microflora. Furthermore, a considerable role in the biochemical consumption of oxygen is played by nitrifying chemosynthetic bacteria. Therefore, in its full version, the complex of full-scale observations of bacterioplankton must include, in addition to the determination of the total number and biomass of bacteria, the quantitative analysis of its various groups.

In the determination of functional parameters of bacterioplankton, main attention should be given to the investigation of the dependence of its growth rate $V_b^{\max}$ on the presence of the nutrient substrate S in water described by the well-known Monod law, which is analogous to the Michaelis–Menten dependence for the rate of photosynthesis. The semisaturation constant Π_S of this law can also be determined on the basis of the graphical solution of a linear equation analogous to (6.11).

An important functional parameter of bacteria is the economic coefficient E, which is a dimensionless constant that characterizes the efficiency of the use of assimilated energy for growth, namely,

$$E = \frac{P_b}{P_b + R_b},$$

where P_b is the production and R_b is the expenditure for the metabolism of bacteria. The second parameter that should be determined is the specific rate of self-oxidation and die-off of bacteria μ_b. It is known that the specific growth rate of bacteria depends on the density of their population. Therefore, it is assumed that

$$\mu_b = \frac{\mu_b B_b}{B_b^{\max}},$$

where $B_b^{\max}$ is the maximum possible concentration of bacterial biomass, which, in particular, can be determined from the empirical dependence [67]

$$\ln B_b^{\max} = 3.88 + 0.36 \ln N,$$

where N is the concentration of saprophytic microflora, cell/ml, and $B_b^{\max}$ is the concentration of raw biomass, mg/ m^3.

Another very important component of the biological part of monitoring is the determination of the rate of biosedimentation at different points of the investigated marine water area because only on the basis of the results of full-scale measurements of the intensity of the flow of organic matter to the bottom sediments can one reliably evaluate the rate of its gravitational settling. For the determination of the rate of biosedimentation, one can use both conventional "sedimentation traps" with subsequent separation of the organic part of the settled suspension and the more modern radiological uranium–thorium method [63, 40].

6.2. Methodological Aspects of the Application of Methods of Mathematical Modeling to the Evaluation of Flows of Pollutants from Bottom Sediments

One of the mechanisms of self-purification of water ecosystems from pollutants of anthropogenic nature is their removal from the circulation in trophic chains and water mass due to processes of gravitational settling of particles of mineral and organic suspension (detritus) followed by their burial in bottom sediments. In this case, pollutants are either initially contained in a suspended organic matter (e.g., biogenic elements or heavy metals accumulated in the biotic component of the ecosystem) or adsorbed by particles of suspension and bottom sediments in the process of their interaction with water.

Detritus, getting into bottom sediments, is partially mineralized. The biogenic elements (including microelements) that are released in this process get into pore water and then into the near-bottom water layer due to the process of molecular diffusion and periodic wind-wave stirring of bottom sediments in shallow water. Since the physicochemical conditions in water mass and in bottom sediments are different, there is a disbalance between the flows of organic matter to bottom sediments and the removal of products of its decomposition into water mass. Furthermore, as a result of changes in physicochemical conditions, the desorption of pollutants from bottom sediments can take place.

Under stationary conditions, the dynamical equilibrium between the contents of pollutants in bottom sediments and in water is established. Therefore, the flows of organic matter to bottom sediments and of products of its decomposition from bottom sediments to water have constant intensities. For the process of sorption, the equilibrium between the concentrations of pollutants in the solid phase and in a solution is described by the equation of Langmuir isotherm [13]:

$$C_s = \frac{C_{s0} bC}{1 + bC}, \qquad (6.17)$$

where C_{s0} is the maximum admissible concentration of the component C_s as $C \to \infty$ (C_{s0} is the capacitance of particles of suspension or bottom sediments) and the coefficient b determines the degree of nonlinearity of the isotherm. However, in practical computations, one more often uses the following special cases of this equation:

(a) the Freundlich equation

$$C_s = k_d C^{1/n} \qquad (6.18)$$

where k_d is the equilibrium constant that characterizes the adsorption force and $1/n$ is the degree of nonlinearity;

(b) the (Henry) equation of linear isotherm

$$C_s = k_d C. \tag{6.19}$$

In the case where the processes running in a basin are quasistationary, the flows of pollutants, which are products of decomposition of organic matter in bottom sediments (mineral compounds of nitrogen and phosphorus, and microelements including heavy metals), can be determined on the basis of the differential equation deduced in [64] and describing the vertical distribution of products of decomposition of organic matter in bottom sediments, namely,

$$D_{es}\frac{d^2C'_s}{dz^2} - w_s\frac{dC'_s}{dz} + K\beta_c C^0_{\text{org}} e^{-K/w_s z} = 0. \tag{6.20}$$

Here, $C'_s(z)$ is the concentration of the considered product of decomposition of organic matter expressed as its mass per unit volume of water-saturated porous sediment, z is the depth of bottom sediments (the $0z$-axis is directed downwards), $D_{es} = D_0 p^2$ is the effective diffusion coefficient of the component in a porous medium, p is the porosity of bottom sediments, D_0 is the coefficient of molecular diffusion of substance in water, w_s is the rate of accumulation of sediments, K is the specific rate of decomposition of organic matter of bottom sediments, C^0_{org} is the concentration of the original organic matter at the surface of bottom sediments, and β_c is the stoichiometric coefficient used for the representation of the concentration of organic matter in the units of one of its components.

The solution of Eq. (6.20) with the boundary conditions $C'_s(0) = C'_{s0}$ and $C'_s(\infty) \le \text{const} < \infty$ has the form

$$C'_s(z) = C'_{s0} + \frac{w_s^2\beta_c C^0_{\text{org}}}{(D_{es}K + w_s^2)(1 - e^{-K/w_s z})}. \tag{6.21}$$

If one knows the values of the concentration of products of decomposition of organic matter $C'_s(z_1) < C'_s(z_2) < C'_s(z_3)$ in the water-saturated porous deposition of bottom sediments at some depths $z_1 < z_2 < z_3$ of the ground monolith, then, using relation (6.21), one can deduce a computation formula for the evaluation of diffusive flow through the water–bottom boundary, namely

$$Q_{w-s} = -\frac{D_{es}\xi[C'_s(z_1) - C'_s(z_2)]}{e^{-\xi z_2} - e^{-\xi z_1}}, \tag{6.22}$$

and a formula for the determination of the constant (specific rate) of decomposition of organic matter in bottom sediments:

$$K = \frac{\xi^2 D_{es}[C_s'(z_2) - C_s'(z_1)]}{\beta_c C_{\text{org}}^0 (e^{-\xi z_1} - e^{-\xi z_2}) - [C(z_2) - C(z_1)]}. \tag{6.23}$$

In relations (6.22)–(6.23), the value $\xi = K/w_s$ is determined either graphically or by selection from the following transcendental equation:

$$\frac{C_s'(z_3) - C_s'(z_1)}{C_s'(z_2) - C_s'(z_1)} = \frac{e^{-\xi z_1} - e^{-\xi z_3}}{e^{-\xi z_1} - e^{-\xi z_2}}. \tag{6.24}$$

If, in addition, one takes into account the adsorption of the considered components on the solid substance of the skeleton of bottom sediments governed by the linear Henry law, then the term w_s^2 in the denominator of relation (6.21) has the factor $(1 + k_d)$, where k_d is the adsorption constant:

$$C_s'(z) = C_{s0}' + \frac{w_s^2 \beta_c C_{\text{org}}^0}{[D_{es}K + (1 + k_d)w_s^2](1 - e^{-K/w_s z})}. \tag{6.25}$$

In this case, one can also perform computations by using relations (6.22)–(6.24) [64].

Thus, the flow of one of the products of decomposition of organic matter can be determined on the basis of data of discrete measurements of its concentration in the pore solution at three depths of the ground monolith. Prior to the application of relations (6.22)–(6.24), one should recalculate these concentrations in terms of their values in the water-saturated porous sediment by multiplying them by porosity. Samples are taken from the upper 10 cm layer of bottom sediments.

However, there is another method for the evaluation of the flows of components of organic matter through the water–bottom boundary by using the solution of equations of macrokinetics in bottom sediments, which is based on the measurement of the rate of accumulation of sediments w_s in the basin. In this case, the total flow of a biogenic element through the surface of bottom sediments can be computed by the relations [64]

$$Q_{w-s} = -\frac{D_{es} K w_s \Re_0}{D_{es}K + w_s^2} + w_s C_{s0}' \tag{6.26}$$

or, with the use of the adsorption process,

$$Q_{w-s} = -\frac{D_{es} K w_s \Re_0}{D_{es}K + w_s^2(1 + k_d)} + w_s(1 + k_d)C_{s0}', \tag{6.27}$$

where $\Re_{s0}$ is the concentration of organic matter at the water–bottom interface in units of the biogenic element and C'_{s0} is the concentration of the element (in the mineral form) at the interface. For the value of w_s known from observations, the value of K can approximately be evaluated by using the relation $K = 0.012\, w_s$ (where $[K]$ = day^{-1} and $[w_s]$ = cm/day). If the concentration of the inorganic compound of the biogenic element is known at a certain depth of bottom sediments with coordinate z_*, then the quantity K can be determined from the transcendental equation

$$e^{-K/w_s z_*} = \frac{[C'_{s0} - C(z_*)][D_{es}K + w_s^2]}{w_s^2 \Re_{s0}} + 1$$

or

$$e^{-K/w_s z_*} = \frac{[C'_{s0} - C(z_*)][D_{es}K + (1 + k_d)w_s^2]}{w_s^2 \Re_{s0}} + 1.$$

Note once again that the relations presented above are obtained under the assumption that the processes running in the water ecosystem are stationary. At temperate latitudes, the chemical and biological processes can only be considered as stationary if they are averaged over a year. This is explained by the substantial influence of the temperature of the medium on the rate of these processes. It is clear that, during a year, the rate of primary production of organic matter by autotrophs and the rate of biosedimentation (and, hence, the content of organic matter at the water–bottom interface) are changing. On the other hand, it is known that, as a rule, the rate of accumulation of sediments in the shelf zone of the sea and water basins does not exceed the value of several millimeters to one centimeter per year (except for mouth regions). The pore solution is separated from a layer of a ground column several centimeters in height. Thus, the accuracy of sampling of pore water from a ground column aimed at the determination of the content of organic matter and products of its decomposition at the water–bottom interface automatically provides the stationarity of flows whose values are computed on the basis of the relations presented above.

An increase in the accuracy of the determination of boundary values of these characteristics enables one to investigate the seasonal variability of the values of flows.

It is reasonable to apply the method described above to the determination of the flows of pollutants in the case where the organic matter of detritus is their main source in bottom sediments. However, there is a strong reason to suppose that, for some pollutants, the processes of their sorption and desorption by organic and mineral particles of bottom sediments prevail in the formation of flows through the water–bottom interface. In this case, for the computation of the value of the flow, we can use the following relation [38]:

$$Q_{\text{sed-w}}^{\text{sorb}} = (1 - p)d_s \nu_{\text{sed-w}}(k_d C - C_s), \tag{6.28}$$

where $Q_{\text{sed-w}}^{\text{sorb}}$ is the sorption flow of pollutants through the bottom–water interface, $\text{mg/m}^2\text{day}$, p is the porosity of bottom sediments, d_s is the mean diameter of particles, m, $\nu_{\text{sed-w}}$ is the constant of intensity of sorption exchange in the "water–bottom sediments" system, day^{-1}, k_d is the coefficient of equilibrium distribution for the indicated system according to the Henry law, C is the concentration of pollutants in the dissolved form in the near-bottom water layer, mg/m^3, and C_s is the concentration of pollutants in bottom sediments.

Possible changes in the direction of the sorption exchange of pollutants between water and bottom sediments are taken into account in relation (6.28). In the case where the equilibrium concentration of pollutants in bottom sediments $C_s^R = k_d C$ determined on the basis of the equation of linear isotherm in terms of the concentration of pollutants in near-bottom water C is greater than the measured quantity C_s, this substance is sorbed by particles of bottom sediments. Otherwise, the desorption process occurs. This result is very important for the investigation of the role of bottom sediments as a source of repeated pollution of marine environment.

If one assumes that, on the scale of an average statistical annual cycle, an equilibrium is established between the contents of a pollutant in water and in bottom sediments in the water–bottom sediments system, then the interannual oscillations of the content of this substance in water related, e.g., to the variability of the river discharge or the intensity of wind-wave stirring of bottom sediments in shallow water can lead to the situation where bottom sediments become sources of the inflow of pollutants to the water medium. The probability of the appearance of this process is determined by the sorption capacitance of particles of bottom sediments, which, in turn, is characterized by the value of the equilibrium constant k_d. If, for a given type of bottom grounds, the value of k_d is determined from a laboratory experiment, then, on the basis of the observation data on the variability of the concentration of a pollutant of the investigated type in near-bottom water and its content in bottom sediments, one can make a conclusion about the possibility of the appearance of the phenomenon of desorption and evaluate the assimilation capacitance of bottom sediments for the investigated type of pollutants.

The main problem in the computation of sorption flows of pollutants at the water–bottom interface is the determination of the value of the coefficient k_d. It can be directly determined in laboratory experiments [29] or calculated on the basis of empirical dependences that generalize the data of laboratory experiments performed by different researchers [140].

Laboratory experiments aimed at the determination of the coefficient k_d are carried out in two ways. In the first case, different samples of bottom sediments are added to water with known concentration of pollutants. Then the dynamics of the adsorption of pollutants by particles of the ground is observed up to reaching the equilibrium of the concentrations in the water–suspension system. In the second case, bottom sediments with known content of pollutants are placed at the bottom of an aquarium filled with pure water. Adding different amounts of a pollutant to the water of the aquarium, one monitors the variation in its concentration in the solution and determines the concentrations corresponding to the equilibrium in the investigated system. The result of experiments of this kind is an adsorption isotherm (and, hence, the value of k_d) and the time curves of the concentrations of pollutants in the solution reaching the equilibrium mode. On the basis of these curves, one determines the value of $\nu_{\text{sed-w}}$ in relation (6.28).

In the computation of the equilibrium constant k_d on the basis of empirical dependences, one uses information on specific features of their chemical composition [145], e.g., on the content of organic matter in bottom sediments.

Finally, note that, in special literature, the concentration C of a pollutant in a solution in dependences of the form (6.18) and (6.19) is measured, as a rule, in mg/m^3, C_s is measured in mg of the pollutant per unit mass of the ground (e.g., mg/g), and k_d is measured in m^3/g. However, in relations (6.25) and (6.27), C_s' is determined in units of mass of the pollutant per unit volume of a water-saturated porous sediment. Therefore, prior to using these relations, one should multiply k_d by the density of the water-saturated porous sediment.

Further, we dwell on another aspect related to the estimation of the role of bottom sediments as a source of repeated pollution of marine environment.

It is known that, in the zone of near-shore shallow water where the depth does not exceed half length of a wind wave, strong winds cause stirring of bottom sediments. In this case, polluted pore waters of a turbid layer of bottom sediments arrive at the overlying water column. Furthermore, one may expect the desorption of pollutants from the suspension of turbid bottom sediments and the transition of these substances into a dissolved state. At present, there are no estimates for the role of this mechanism in the repeated pollution of water by bottom sediments of the near-shore zone of the sea.

The main problem here is the determination of the amount of suspension getting into water and, hence, the thickness of the turbid layer of bottom sediments for a given force of wind and a given depth.

The thickness of the turbid layer can be calculated if one knows the total amount of suspension getting into a water column from bottom sediments:

$$\xi_s = \frac{S_\Sigma}{(1-p)\rho_s}, \tag{6.29}$$

where ξ_s is the thickness of the perturbed layer of bottom sediments, S_Σ is the total amount of suspension in a water column of height H coming from bottom sediments, and ρ_s is the density of particles of the suspension.

For the computation of the quantity S_Σ, we use the conclusions of the mathematical model of formation of a vertical profile of concentration of suspended silt described in [8] and obtain the following relation for the vertical distribution of the concentration S of suspended silt:

$$\begin{aligned} S &= S_e \exp\left(-\frac{w_b}{\varepsilon_1} z\right) \quad \text{for} \quad z \le \delta_0, \\ S &= S_e \exp\left(-\frac{w_b \delta_0}{\varepsilon_1}\right)\left(\frac{z}{\delta_0}\right)^{-w_s\delta_0/\varepsilon_1} \quad \text{for} \quad z > \delta_0, \end{aligned} \tag{6.30}$$

where S_e is the near-bottom concentration of silt determined by the empirical dependence

$$S_e = 0.035\left(\log\frac{u_{*m}}{w_b}D_*^{0.7}\right)^{3.75}, \tag{6.31}$$

z is the vertical coordinate directed from the bottom to the surface, w_b and w_s are the hydraulic sizes of bottom silt and suspended silt, respectively, δ_0 is the thickness of the near-bottom layer, namely

$$\delta_0 = \frac{\sqrt{2}\pi H\varepsilon_1}{u_m^2\tau\left(\frac{sh(2kH)}{4kH}-\frac{1}{2}\right)}, \tag{6.32}$$

$k = 2\pi/\lambda$, λ is the length of the wind wave, τ is the period of the wind wave, u_{*m} is the maximum value of friction velocity in the wave flow, i.e.,

$$u_{*m} = \frac{\chi u_m}{\ln\left(1.6\frac{a_\delta}{k_s}+1\right)}, \tag{6.33}$$

$k_s = 2.5d_{sr}$, d_{sr} is the mean diameter of bottom silt, $\chi = 0.4$ is the Kárman constant,

$$a_\delta = \frac{u_m}{\omega},$$

$\omega = \frac{2\pi}{\tau}$ is the angular frequency of surface waves,

$$u_m = \frac{\pi h_w}{\tau sh(kH)}$$

are the maximum orbital velocities near bottom in the wave flow, h_w is the height of the surface wave, ε_1 is the diffusion coefficient in the near-bottom layer calculated according to the empirical dependence

$$\varepsilon_1 = 0.27u_{*p}\frac{u_m\tau}{2\pi}\left(\frac{w_b}{u_{*p}}\right)^{3.32}\frac{gd_{sr}(s-1)}{w_b^2} \quad \text{for} \quad \frac{w_b}{u_{*p}} < 0.52,$$

$$\varepsilon_1 = 0.44u_{*p}\frac{u_m\tau}{2\pi}\left(\frac{w_b}{u_{*p}}\right)^{0.51}\frac{gd_{sr}(s-1)}{w_b^2} \quad \text{for} \quad \frac{w_b}{u_{*p}} \geq 0.52, \tag{6.34}$$

u_{*p} is the amplitude of the friction velocity in the wave flow for the grain roughness calculated by (6.33) for $k_s = 2.5d_{sr} + \Delta$, Δ is the height of bottom riffles, $s = \rho_s/\rho$ is the relative density of the bottom ground, and ρ_s and ρ are the densities of suspension and water, respectively.

The values of w_b and w_s can be calculated by using the well-known Stokes expression or more universal dependences [27] in terms of the density and mean diameter of bottom silt d_{sr} and suspended silt $d_{sus} = d_{sr}(1 - 0.7\exp(-0.3T_m))$, namely,

$$T_m = \frac{u_{*m}^2}{u_{*\mathrm{cr}}^2} - 1,$$

where $u_{*\mathrm{cr}}^2$ is the critical friction velocity corresponding to the beginning of the motion of silt, namely,

$$u_{*\mathrm{cr}}^2 = gd_{sr}(s-1)\theta_{\mathrm{cr}}, \tag{6.35}$$

$$\theta_{\mathrm{cr}} = 0.24D_* \quad \text{for} \quad D_* \le 4,$$

$$\theta_{\mathrm{cr}} = 0.14D_*^{-0.64} \quad \text{for} \quad 4 < D_* \le 10,$$

$$\theta_{\mathrm{cr}} = 0.04D_*^{-0.1} \quad \text{for} \quad 10 < D_* \le 20,$$

$$\theta_{\mathrm{cr}} = 0.013D_*^{0.29} \quad \text{for} \quad 20 < D_* \le 150,$$

$$\theta_{\mathrm{cr}} = 0.055 \quad \text{for} \quad D_* > 150,$$

$$D_* = d_{sr}\left[\frac{g(s-1)}{\nu^2}\right]^{1/3}$$

g is the acceleration of gravity, and ν is the coefficient of molecular kinematic viscosity of water.

Integrating expressions (6.30) within the limits of the corresponding water layers and summing them up, we obtain the following relation for S_Σ:

$$S_\Sigma = \int_0^{\delta_0} S\,dz + \int_{\delta_0}^{H} S\,dz = C_a\left[\frac{\varepsilon_1}{w_b}(1-e^{-\gamma}) + e^{-\gamma}\frac{\delta_0}{1-\gamma_s}\left(\left(\frac{H}{\delta_0}\right)^{1-\gamma_s} - 1\right)\right], \tag{6.36}$$

where

$$\gamma = \frac{w_b}{\varepsilon_1}\delta_0 \quad \text{and} \quad \gamma_s = \frac{w_b}{\varepsilon_1}\delta_0.$$

Then the mean content of suspension in a water layer of thickness H is equal to $\bar{S} = S_\Sigma / H$. Following [38], one can calculate the sorption flow of pollutants in the "water–suspension" system by relation (4.5).

The amount of pollutants getting into a water column together with pore water due to wind-wave stirring of bottom sediments can be estimated as follows:

$$M_c = \rho_{sw}\xi_s\Omega p C_s^p, \tag{6.37}$$

where ρ_{sw} is the density of the water-saturated porous sediment, kg/m^3, C_s^p is the concentration of pollutants in pore water of bottom sediments, mg/m^3, and Ω is the area of the bottom, m^2, that is the base of the water column receiving the pollutants that were earlier contained in the pore water of the turbid layer of bottom sediments of thickness ξ_s. The increment ΔC, mg/m^3, in the concentration of a pollutant in a water column with unit base and height H, m, is equal to

$$\Delta C = \frac{\rho_{sw} p \xi_s C_s^p}{H}. \tag{6.38}$$

The initial data for relations (6.29)–(6.38) are the measured or calculated characteristics of wind waves at a local point of coastal shallow water for a given force of wind.

Conclusions

The main requirements for the data obtained in the process of ecological monitoring of marine water areas imposed by the necessity of its further use in ecosystems analysis and the construction and calibration of mathematical models of water quality and operation of water ecosystems are the following:

— the integrality of the system of observations and experiments, which enables one to establish cause-effect relationships in the dynamics of elements of the ecosystem and their dependence on the characteristics of water medium;

— the system of monitoring must be organized so as to not only monitor the characteristics of the current state of the ecosystem, but also to include specialized observations and full-scale and laboratory experiments necessary for the development of the concept, calibration of parameters, and verification of developed models.

In the course of specialized observations and experiments, one determines parametric characteristics of the flows of substances and energy between elements of the ecosystem and their dependence on current and mode hydrological, chemical, and biological characteristics of the water medium.

The experimental determination of typical values of parameters of mathematical models of water ecosystems and ranges of their actual variability is a complicated scientific problem that requires an individual methodological approach in each individual case. The values of many parameters cannot be directly measured, and, for their indirect estimation on the basis of the results of observations and experiments, one uses elements of mathematical modeling. The determination, systematization, and development of these methods are of major scientific and practical interest because they enable a broad circle of users to use mathematical models of water quality and operation of water ecosystems. This problem has been solved in this chapter. In particular, we have considered the methodological aspects of determination of specific rates of production, eating away, and mortality of phytoplankton, mineralization and biochemical oxidation of organic matter, nitrification, etc., and generalized, in the form of methods, the conclusions of mathematical models made in different works that enable one to evaluate the flows of pollutants between water and bottom sediments for the determination of their role as a potential source of repeated pollution of water objects.

7. DETERMINATION OF THE STRATEGY OF CONTROL OF WATER QUALITY OF MARINE WATER AREAS

The development and modification of the methodology of application of mathematical water-quality models to the solution of applied problems of marine nature management is a problem no less urgent and complex than the development of the structure and calibration of these models. This is explained by the fact that, despite the complexity of the mathematical structure and numerical realization of contemporary water-quality models, they are not universal because of the diversity of considered applied problems and types of pollutants and their properties, and the diversity and variability of natural and anthropogenic factors that form the quality of the habitat of hydrobionts and specific features of operation of water ecosystems.

Water-quality models describe only the most important elements of ecosystems and chemical and biological processes connecting them in the water medium. The application of a model and its information possibilities are restricted by assumptions and simplifications used in their development. The neglect or ignorance of them can lead to a wrong interpretation of obtained results and their inadequacy or triviality. The correct and efficient application of mathematical water-quality models to the solution of applied problems depends on the systematic knowledge of physical, chemical, and biological processes running in the marine medium and their correlation.

On the other hand, the more complicated the structure of a model, the more data are necessary for its qualitative calibration, verification, and application. This leads to a considerable increase in requirements and financial expenditures necessary for the ecological monitoring of the modeled ecosystem, as a result of which the project may become economically unprofitable.

As a rule, a researcher deals with the following problem: Using a mathematical model, give scientifically substantiated practical recommendations for ways of realization of economic or nature-management projects, minimizing the requirements on support and expenditures for ecological monitoring.

Thus, the development of methods and procedures for the application of relatively simple (from the viewpoint of operation of an actual ecosystem) mathematical water-quality models for the efficient and adequate solution of applied problems of marine ecology is of indisputable scientific and practical interest.

The aim of the present chapter is to illustrate the possibilities and methodology of application of numerical mathematical water-quality models to the solution of applied problems of sea ecology associated with the choice of optimal strategy of marine nature management and the preservation and restoration of the quality of water medium.

7.1. Development of Recommendations for the Improvement of Hydrological and Hydrochemical Modes of the Tuzla Group of Firths

The results of computation of the water-salt balance in the Tuzla group of firths and historical experience [85, 87] show that the present-day mode of their fish-economic use (according to which several artificial channels connecting the firth with the sea are made in a sand bay bar (these channels are opened in spring for fish access and in summer for fish catching)) facilitates a control over the ecological state of the basin, enabling one to avoid negative consequences of its shallowing and salinization. Through these channels, the basin is artificially filled with seawater, which facilitates the relative "desalination" of firth waters in autumn and, in low-water years, in spring. Moreover, under conditions of a mean-water year, the amount of salts removed from firths during spring water exchange with the sea is greater than the amount of salts arriving with seawater in autumn [22]. In the course of filling of the basin in spring and autumn, its biological "revival" occurs, whereas in summer, at the minimum level checkmarks in the period of isolation of the basin, water quality and conditions for the existence of higher hydrobionts deteriorate [91].

On the other hand, as indicated in Sec. 2.2.2, under the conditions of the present-day scheme of fish and water management of the Tuzla firths, their actual fish productivity is less than their potential and continues to decrease. For this reason, there arises the problem of reconstruction of hydrological and hydrochemical modes of firths by providing their continuous water exchange with the sea in summer via permanently operating artificial passages in the bay bar. It is assumed that, as a result of an increase in water renewal and the relative stabilization of water level, the temperature and salinity modes and the water quality of firths approach the marine ones and become suitable for the reproduction of numerous species of fish and other hydrobionts encountered in the adjacent marine water area.

Thus, the problem of control of water quality of the ecosystem of the Tuzla group of firths reduces to the determination of the optimal number of artificial passages in the spit and their location for providing the maximum water exchange with adjacent marine water area. This problem can be solved on the basis of the hydrodynamic model described in Chap. 3.

At time scales of the order of a natural synoptic period, the intensity of water exchange between the firths and the open sea is determined by wind-surge oscillations (denivellations) of the water level. In this case, the water flow in channels is guaranteed by different types of wind denivellations of the water level in the Tuzla water basin and in the adjacent marine water area. Therefore, for the correct description of the influence of wind-surge phenomena on the water exchange through narrow passages in the bay bar, the computational region must include not only the water area of firths but also the adjacent region of the sea.

At the first stage, the hydrodynamic model was used for the investigation of specific features of circulation of water and wind-surge oscillations of the water level in firths and in the adjacent region of the sea for the determination of sections of the bay bar for which, in the wind mode typical of the region, the difference between the water levels in the firth and in the sea is maximum for the most part of time.

In computation, the water area of the Tuzla firths was covered by a computational grid with 65×22 nodes with step 500 m. With regard for small depths, four computational levels along vertical line were used.

The second computational region was the water area of the west part of the northwest shelf of the Black Sea with south boundary along 45°00′ N and east boundary along 31°10′ E (Fig. 7.3). This water area was covered by a computational grid with 62×93 nodes with step 2000 m. Ten computational levels along the vertical line were used. The influence of the Danube discharge on the denivellation of the sea level and the formation of discharge (gradient) currents in the part of the computational region adjacent to the Tuzla firths was taken into account. It was assumed that the total discharge rate of the Danube through all its armlets is constant and equal to 6460 m^3/sec.

Computations were carried out for stationary winds of eight main directions, namely N, NE, E, SE, S, SW, W, and NW, with velocities of 5 and 8 m/sec. As expected, the maximum differences between the levels of water surfaces were observed for longitudinal NE and SW winds relative to the axis of the Tuzla basin, and the minimum ones were observed for transverse NW and SE winds (Fig. 7.1). For wind velocities of 5 m/sec, the maximum difference between the water levels of the south and the north boundaries of the basin was equal to $\approx$ 10 cm, whereas, as the wind velocity increased to 8 m/sec, the maximum difference became greater than 30 cm. On the whole, the N, NE, E, S, SW, and W winds, which led to pronounced differences between the water levels of the south and the north parts of the basin along the marine spit, were observed in summer in 70–80% of cases according to the data of [21] and of the Ust'-Dunaisk Hydrometeorological Station.

The specific feature of the integral wind circulation of waters in the basin is the intensive water exchange between the Shagany Firth and the Alibei Firth via their common lower part adjacent to the marine bay bar. On the contrary, the water exchange between the Burnas and Karachaus firths and the other part of the basin is hampered (Fig. 7.2).

Computations for the region of the northwest shelf of the Black Sea adjacent to the Tuzla group of firths showed that the denivellations of the sea level are determined by the interaction of wind and discharge currents (Fig. 7.3). For light winds, due to the influence of river discharge, the sea level is always higher than or equal to the water level in firths. Only for wind velocities of up to 8 m/sec may slight surges be observed for W and NW winds on the seaside of the Tuzla bay bar. Furthermore, for winds of equal velocity, the amplitude of oscillations of the water level in the sea is smaller than that in the basin. This difference increases significantly with wind velocity. For example, for a wind velocity of 8 m/sec, the maximum difference in water levels in the firth can reach 30 cm, whereas, at the seaside, the difference in water levels along the spit does not exceed several centimeters and the amplitude of oscillations of the level does not exceed 7 cm for winds of different directions.

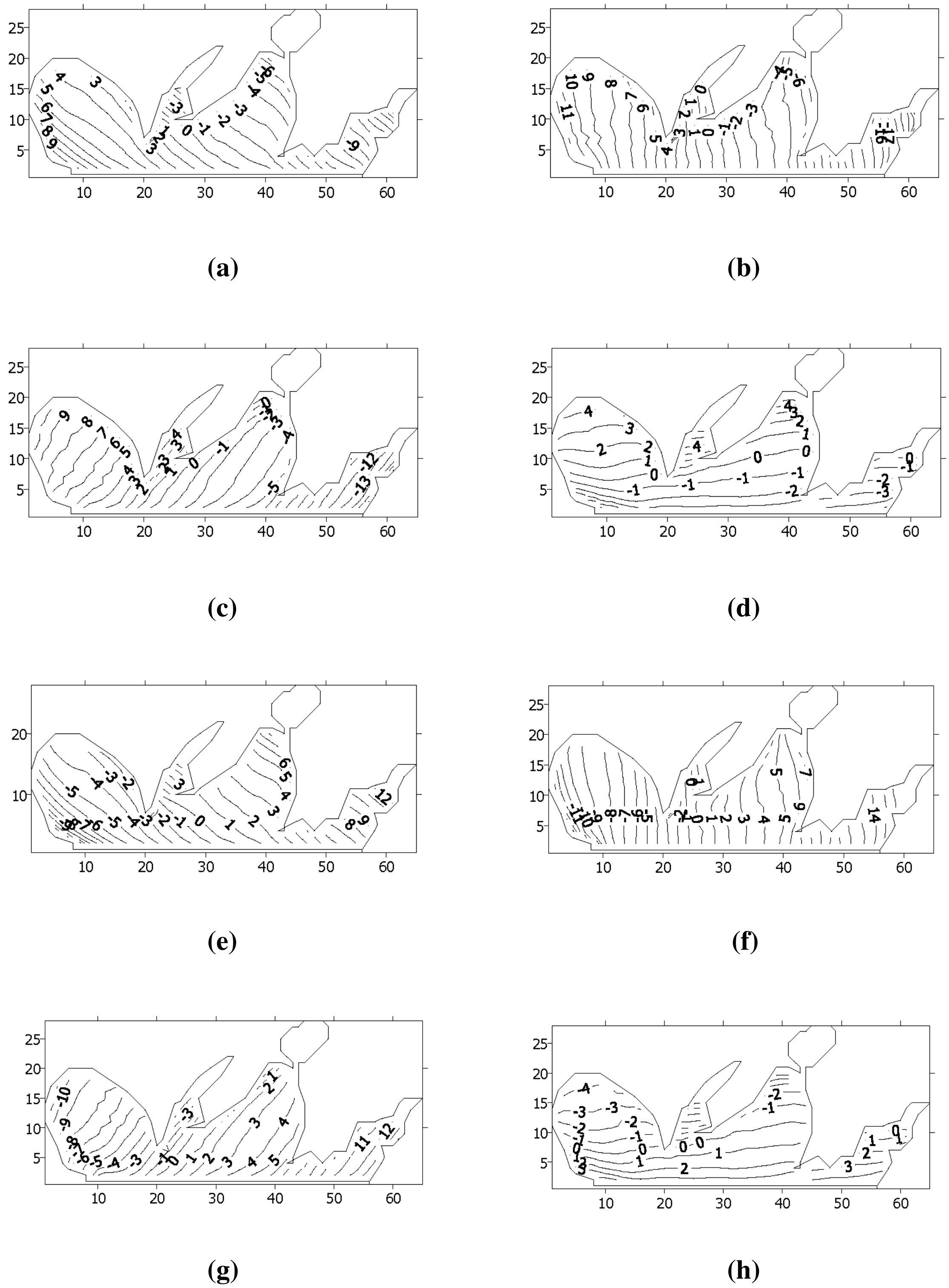


Fig. 7.1. Denivellation (in cm) of the sea level in firths for a wind with velocity of 8 m/sec and directions N (a), NE (b), E (c), SE (d), S (e), SW (f), W (g), NW (h).

Thus, the results of computation for the circulation of waters and denivellations of the water surface for winds of different directions and velocities performed by using the hydrodynamic model show that the location of connecting channels in the north and south parts of the sand bay bar is optimal for providing the maximum water exchange with the sea and the renewal of waters of the Tuzla basin. In 70–80% of wind cases, a significant difference between the levels of the water surface occurs between these points of the basin. Furthermore, the basin can be conditionally divided into two parts (Burnas and Shagany–Alibei) the water exchange between which is hampered. As a result, the maximum values of salinity are observed in the Burnas Firth. Therefore, in order that water renewal be guaranteed in both parts of the basin, each part must have a connecting channel.

For the verification of these reasonings based on the computation of the circulation of waters and wind denivellations of the water surface in firths, numerical experiments were carried out on the basis of the hydrodynamic model. In these experiments, the salinity of water in the Tuzla firths was used as a passive conservative tracer of waters and an index of efficiency of various management and engineering solutions. A simplified version of the model that takes into account only wind and discharge currents was used.

The modeling of the water and salt exchange between the Tuzla firths and the sea was carried out on May 1–September 30 under wind conditions of 2002 according to the Ust'-Dunaisk hydrometeorological station. The velocity and direction of wind were specified every 3 h and were accepted by the model in the process of computation. At the endpoints of the marine boundary, the perturbations of the sea level computed for the same wind conditions according to the model adapted to the water area of the adjacent part of the Black Sea were specified every 3 h. The water salinity at the marine boundaries was assumed to be uniform, and, according to the data of [14], it increased from 12‰ in May to 15‰ in September. According to [85], the initial water salinity (in May) in the Tuzla basin was assumed to be equal to 21‰, and its space distribution in the basin was uniform.

Initially, the dynamics of waters of the firths and the variability of their salinity in May–September was modeled in the absence of water exchange with the sea. It was assumed that, during the computational period, the maximum depth of the basin decreased due to evaporation by 0.9 m as compared with the original depth of 3.4 m at the beginning of May, which corresponds to the situation of an extremely low-water year in the water-balance computation. The results of computation performed on the basis of the hydrodynamic model showed that, under these conditions, the mineralization of waters by the end of September increases to 38.4–37.7‰ in the water area of the Shagany Firth and Alibei Firth and to 43.4 and 43.7‰ in the Karachaus Firth and Burnas Firth, respectively, as compared with spring (21‰), when the natural water exchange with the sea occurs.

To estimate the efficiency of different ways of construction of connecting channels in the sand bay bar that separates the Tuzla firths from the sea, a series of numerical experiments with model was carried out. In these experiments, the distribution of salinity over the water area of the basin was computed in the presence of an artificially provided uncontrolled exchange of water and salt with the sea. The following alternatives were considered:

(1) a single connecting channel 50 m wide located in the north part of the bay bar (Burnas);

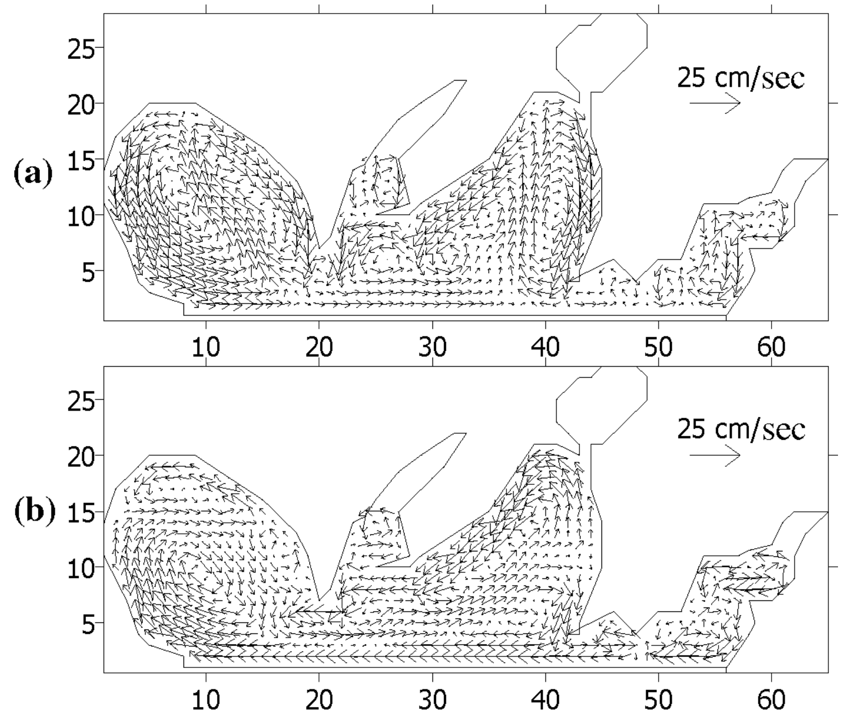


Fig. 7.2. The field of circulation of waters integral over depth in the Tuzla firths for NE-longitudinal (a) and NW-transverse (b) winds with velocity of 8 m/sec.

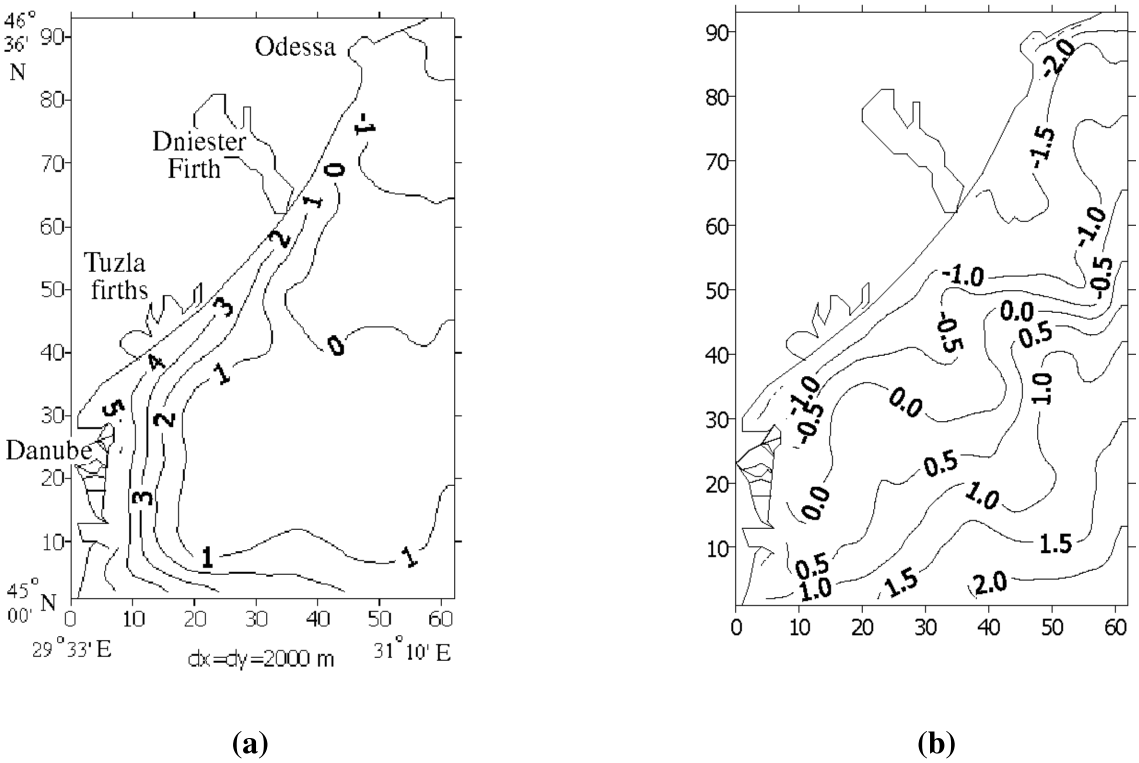


Fig. 7.3. The field of perturbations of the sea level (in cm) in the west part of the northwest shelf of the Black Sea for NE (a) and NW (b) winds with velocity of 8 m/sec.

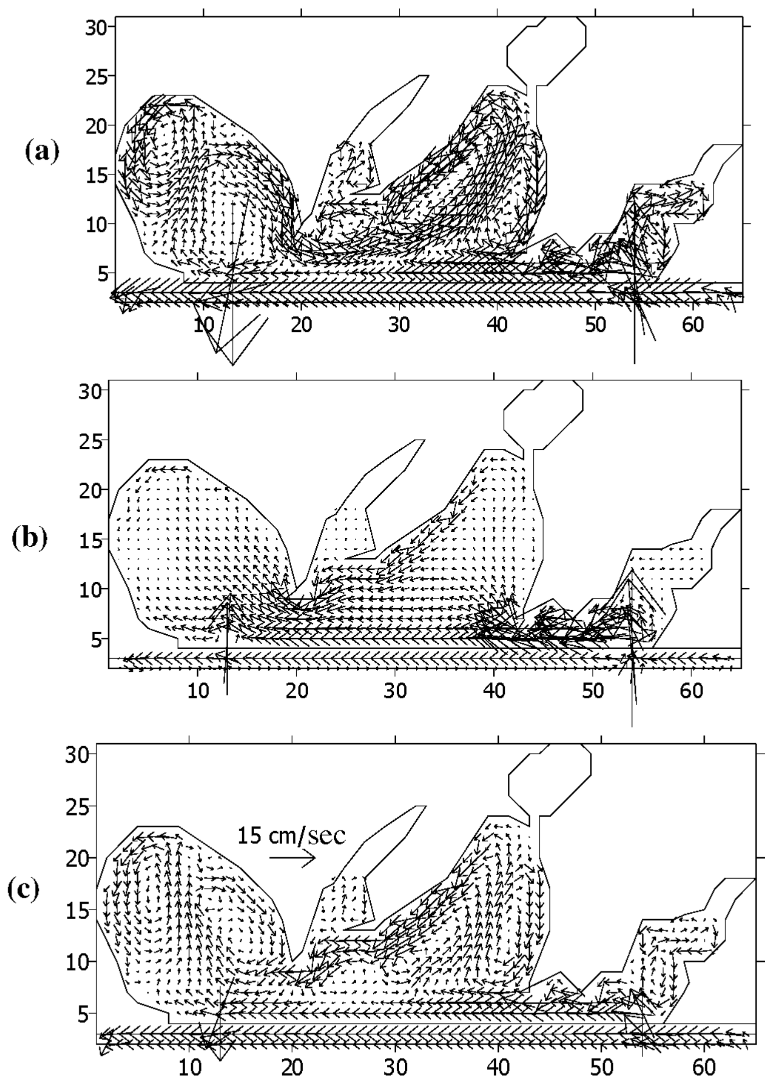


Fig. 7.4. The field of currents integral over depth in the Tuzla firths and in the adjacent marine water area in the presence of connecting channels in the north and south parts of the bay bar corresponding to the data (wind data for 2002) of May 30 (a), July 20 (b), and August 20 (c).

(2) a single connecting channel 50 m wide located in the south part of the bay bar (Shagany);

(3) two connecting channels 50 m wide one of which is located in the central part of the bay bar (Alibei) and the other in its north part (Burnas);

(4) two connecting channels 50 m wide one of which is located in the south part of the bay bar (Shagany) and the other in its north part (Burnas).

In all cases, the water exchange through the channels was not controlled and was provided by denivellations of the sea both in the Tuzla basin and in the adjacent marine water area (Fig. 7.4).

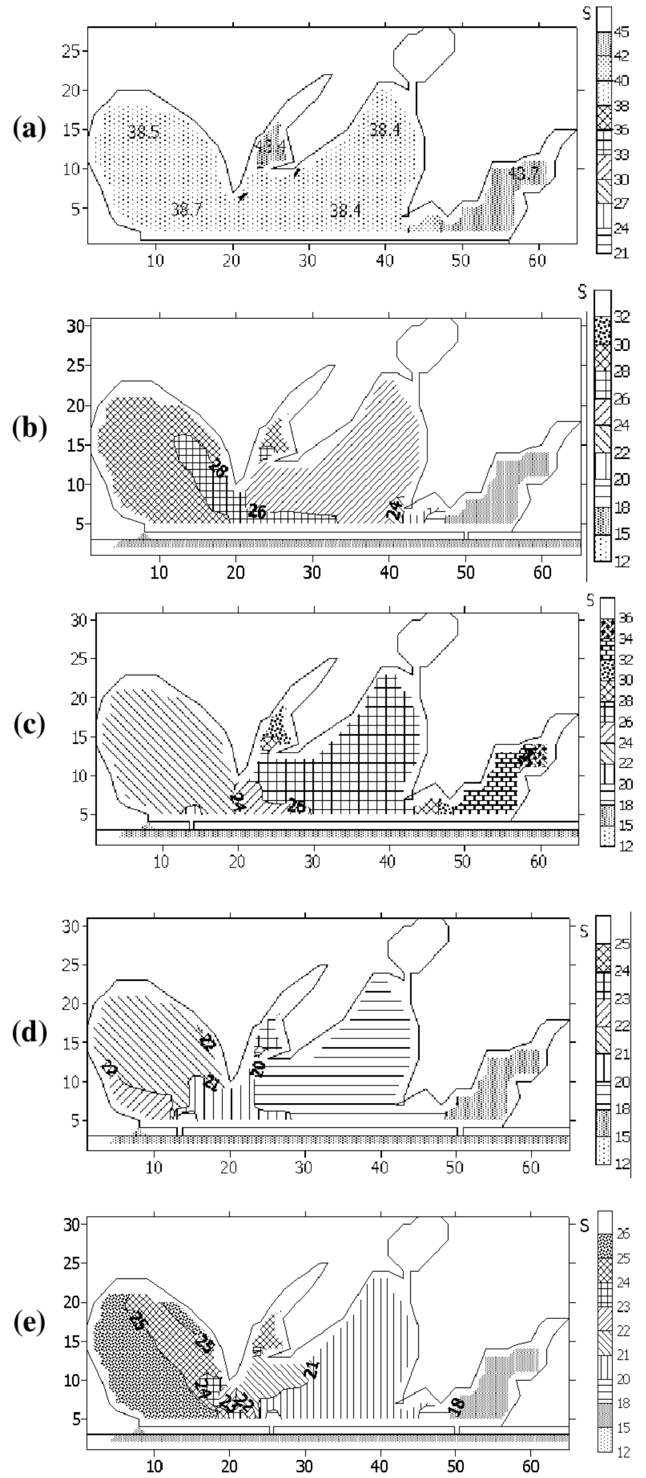


Fig. 7.5. Space distribution of salinity (‰) on September 20 (wind for 2002) computed in the absence of water exchange with the sea (a) and for alternatives 1 (b), 2 (c), 3 (d), and 4 (e).

The results of computation showed that alternative 4 is the most efficient for guaranteeing the maximum water exchange with the sea and the maintenance of the water salinity in the basin at a stable low level. In the case of the realization of this alternative, for the entire computational period the water salinity is minimum (up to 17‰) in the Burnas Firth and maximum (up to 23–24‰) in the Shagany and Karachaus firths (Fig. 7.5e). For channels 50 m wide, the current velocity in a channel reaches 60 cm/sec at certain moments of time (Fig. 7.4).

The shift of the south connecting channel toward the center of the basin (case 3) leads to a decrease in the water exchange with the sea and the water renewal in the Shagany and Karachaus firths, where the mineralization of waters increases to 24–26‰ by the end of the computational period (Fig. 7.5d).

In the case of only one connecting channel in the north part of the bay bar adjacent to the Burnas Firth (case 1), the water salinity in the Shagany and Karachaus firths increases to 28–29‰ (Fig. 7.5b), whereas in the north part of the basin it remains low (up to 18‰).

If a single channel is constructed in the south part of the bay bar adjacent to the Shagany Firth (case 2), then water salinity increases by the end of the computational period to 23‰ in this part of the firth and to 32–36‰ in the Karachaus and Burnas firths (Fig. 7.5c).

In the analysis of the obtained results, the water salinity of the Tuzla firths is considered as an index of water quality of the basin as compared with seawater and as an index of intensity of water exchange with the sea and the water renewal in the firths. Therefore, in case 4, we obtain the maximum washing of the Tuzla firths and renewal of their waters with seawater. In this case, the water quality of the firths is determined by the quality of inflowing seawater.

In the case of a single channel, the water renewal increases if the channel is located in the north part of the spit adjacent to the Burnas Firth. However, in this case, the water in the basin is no longer running, and the basin turns into an accumulator of salt and pollutants inflowing with seawater.

Thus, the results of numerical experiments with hydrodynamic model show that the Tuzla group of firths can be transformed into a partially running-water basin with high level of water renewal and water quality close to that of the sea. This can be realized by the construction of two channels 50 m wide in the sand bay bar at the south (Shagany) and north (Burnas) ends of the sand bay-bar spit. The analysis of the wind dynamics of waters and denivellations of the water level checkmarks in the basin and in the adjacent part of the sea shows that this number and the location of connecting channels are optimal.

7.2. Choice of Location for a Pollution Source According to the Criterion of Minimization of Damage to Marine Ecosystem (by Example of the Odessa Region of the Northwest Part of the Black Sea)

This problem is of undoubted practical importance because it allows one to optimize the location of newly created anthropogenic pollution sources and, in prospect, to organize the operation of already functioning sources so that the concentration of pollutants in nature-conservation areas does not exceed maximum allowable concentrations. For the first time, this problem was considered in [58] for atmospheric pollution sources.

The problem presented below was considered by one of the authors together with S. A. Lonin in [55, 141] in a somewhat different statement: Find a place in the water area of the Odessa region of the northwest part of the Black Sea for the construction of a remote oil terminal complex that is optimal from the viewpoint of minimization of the probable level of pollution of nature-conservation areas of the sea by oil products passing to the marine medium due to technological losses.

In the computation of the fields of pollution caused by technological losses of an oil terminal complex, the following assumptions were made:

— oil products are represented in the form of a water-oil emulsion on the basis of the assumption that small portions of oil rapidly emulsify;

— neglecting evaporation and chemical and biological processes of destruction, we represent an oil product as a conservative passive tracer, which leads to an "upper bound" for the content of oil products in the area of pollution and the use of the strategy of minimum risk in the estimation of damage to the ecosystem.

The transport of oil products is determined by the space field of currents (with regard for the vertical velocity w_0 of floating of oil particles in emulsion) and the intensity of turbulent exchange. The fields of steady currents for typical synoptic situations were preliminarily computed on the basis of the hydrodynamic model [51].

For a semibounded region of the northwest part of the Black Sea, we rewrite Eq. (1.1) in the form

$$BC + LC = f, \tag{7.1}$$

assuming that the oil source f (of power Q) acts permanently and is distributed along the vertical line. In Eq. (7.1), the following notation is used:

$$B = \frac{\partial}{\partial t}, \qquad L = \operatorname{div}(\vec{V}\cdot) + (w + w_0)\frac{\partial}{\partial z} - \alpha_c D_h \Delta - \frac{\partial}{\partial z}\left[\alpha_c (D_\mathrm{v} + \nu)\frac{\partial}{\partial z}\right],$$

Δ is the Laplace operator, D_h is the coefficient of horizontal diffusion, D_v is the coefficient of vertical turbulent viscosity, $\vec{V} = \vec{V}(x, y, z)$ is the three-dimensional vector of components of the current velocity, the $0Z$-axis is directed vertically downward, C is the volume concentration of oil in water, α_c is the inverse turbulent Schmidt factor for suspension, w and w_0 are the vertical velocities of water and particles of emulsified oil drops ($w_0 < 0$), respectively, and ν is the molecular viscosity of water.

Let $C = 0$ at the initial time $t = 0$. At the open sea boundaries $\partial\Omega$ of the considered space region Ω, we set

$$C = 0 \quad \text{at} \quad \partial\Omega \quad \text{for} \quad (\vec{V}\vec{n}) < 0,$$

$$\frac{\partial C}{\partial \vec{n}} = 0 \quad \text{at} \quad \partial\Omega \quad \text{for} \quad (\vec{V}\vec{n}) \geq 0, \tag{7.2}$$

and, for $z = 0$ and $z = H(x, y)$,

$$-w_0 C + (\alpha_c D_\nu + \nu)\frac{\partial C}{\partial z} = 0. \tag{7.3}$$

In Eq. (7.1), the function f has the form

$$f = Q f_1(z)\delta(x - x_0)\delta(y - y_0), \tag{7.4}$$

where $\delta(x)$ is the Dirac delta function, x_0 and y_0 are the coordinates of the source, and the expression for the function $f_1(z)$ is determined from the equilibrium condition

$$D_\nu^{\text{eff}}\frac{\partial C}{\partial z} = w_0 C(z)$$

for the vertical distribution of oil in emulsion [73]. Setting

$$D_\nu^{\text{eff}} = (\alpha_c D_\nu + \nu) \cong \text{const}$$

in this condition for the upper layer and taking into account the entire range of sizes of particles of oil in emulsion in w_0, we get

$$C(z) = C(0) f_1(z),$$

where

$$f_1(z) = \exp\left[\frac{w_0 z}{D_\nu^{\text{eff}}}\right].$$

According to [58], the conjugate problem for C^* on the time interval $t \in [T, 0]$ has the form

$$B^* C^* + L^* C^* = p, \tag{7.5}$$

where

$$B^* = -\frac{\partial}{\partial t},$$

$$L^* = -\text{div}(\vec{V}\cdot) - (w + w_0)\frac{\partial}{\partial z} - \alpha_c D_h \Delta - \frac{\partial}{\partial z}\left[(\alpha_c D_\nu + \nu)\frac{\partial}{\partial z}\right],$$

and p is an arbitrary function. Note that Eq. (7.5) is solved in the case of opposite time direction.

The corresponding boundary conditions following from (7.1)–(7.3) have the form

$$C^* = 0 \quad \text{at} \quad \partial\Omega \quad \text{for} \quad (\vec{V}\vec{n}) < 0,$$

$$\alpha_c D_v \frac{\partial C^*}{\partial \vec{n}} + (\vec{V}\vec{n})C^* = 0 \quad \text{at} \quad \partial\Omega \quad \text{for} \quad (\vec{V}\vec{n}) \geq 0, \tag{7.6}$$

$$w_0 C^* + (\alpha_c D_v + \nu)\frac{\partial C^*}{\partial z} = 0 \quad \text{for} \quad z = 0 \quad \text{and} \quad z = H(x, y), \tag{7.7}$$

$$C^*(x, y, z, T) = C^*(x, y, z, 0).$$

Consider the dual representation of a functional [58]:

$$J \equiv \int_0^T dt \int_\Omega pC\, d\Omega = \int_0^T dt \int_\Omega fC^*\, d\Omega. \tag{7.8}$$

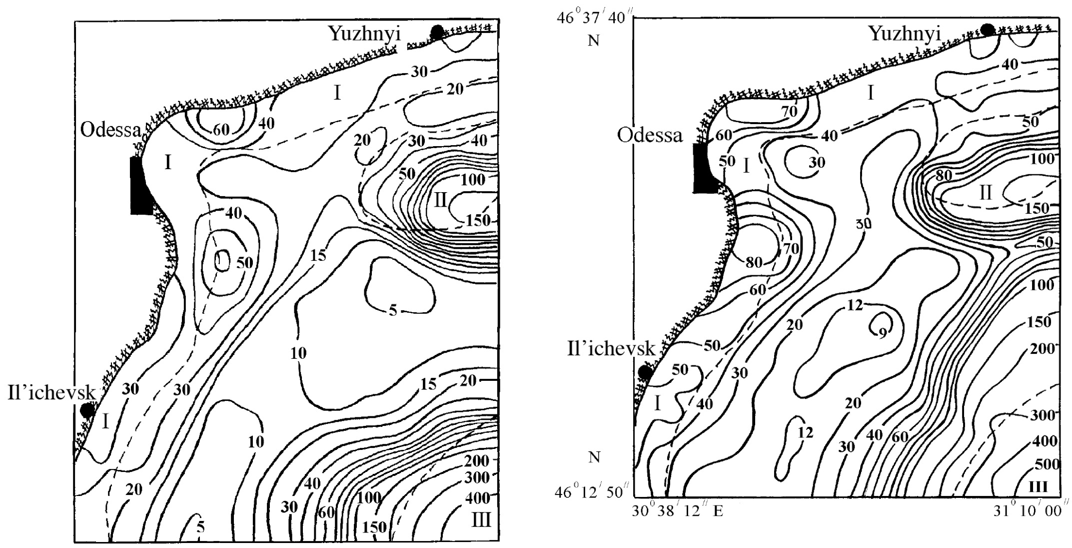
If the functional J has the sense of the level of pollution of seawater by oil products, then, on the basis of its minimum value in the domain Ω, one can determine the optimal area for the location of an oil terminal complex. The use of the left-hand side of equality (7.8) for this purpose requires the multiple solution of the direct problem (7.1)–(7.4) with exhaustion of all possible locations (x_0, y_0) of the source, whereas, on the basis of the right-hand side of this equality, we can obtain the required result using a single solution of the boundary-value problem (7.5)–(7.7).

As an optimization criterion, we take the prevention of pollution in the following nature-conservation areas Ω_+: the four-kilometer near-shore area of the northwest part of the Black Sea, the Zernov phyllophorous field, and the region of the Odessa sand-bank (Fig. 7.6). Taking into account that, under equilibrium conditions, the main part of emulsion is concentrated in the upper water layer, we take the five-meter water layer (H_+ = 5 m). as a nature-conservation region with surface area S_+

We define a function $p(x, y, z)$ as follows:

$$p(x, y, z) = \begin{cases} (S_+ H_+ T)^{-1}, & (x, y, z) \in \Omega_+, \\ 0, & (x, y, z) \notin \Omega_+. \end{cases} \tag{7.9}$$

Then, according to the left-hand side of (7.8), the value of the functional J at every point of the domain Ω characterizes the content of oil products averaged over time T in the five-meter layer of the nature-conservation areas Ω_+, provided that the oil terminal complex is located at this point.



(a) **(b)**

Fig. 7.6. Distribution of the quality functional J (in units of C corresponding to $Q = 1$ c.u./sec) for northwest wind (a) and maximum values of J at every calculated point (b). Dashed lines correspond to the boundaries of the nature-conservation areas (I–III).

The physical meaning of the realization of the conjugate problem is the following: Assume that, under the infinitely long action of a source of power Q, oil has been spread in a finite domain Ω. This result can be obtained by solving the direct problem (7.1)–(7.3). In the solution of the conjugate problem (7.5)–(7.7) with a function p of the form (7.9), the "contraction" of the solution in the opposite direction occurs. Different points of the domain Ω are characterized by different influences of the pollution source on the solution in the nature-conservation area Ω_+. The value of the functional J characterizes this influence at every point of the domain Ω. The points that correspond to the domains of a minimum of the functional J are optimal for the location of an oil terminal complex.

The main factor that determines the water circulation in the northwest part of the Black Sea is a wind. The time of the rearrangement of circulation systems under a change in synoptic situation is small as compared with the time of the action of atmospheric processes of specific type. Since the duration of a change in a synoptic situation does not exceed several hours, and the duration of a synoptic situation is a natural synoptic period (several days), the entire process (under the additivity assumption) can be regarded as continuous in time with arbitrary alternation of meteorological situations of various types. In this case, we can divide the entire investigated period of time into a series of intervals of length T and solve N problems of the form (7.5)–(7.7). The final result can be obtained as the intersection of N ranges of values of the functional J determined for individual typical cases.

The computational region of the northwest part of the Black Sea (46°12′50″–46°37′40″ N, 30°38′12″–31°10′00″ E) was covered by a uniform horizontal grid with step 1 km; along the vertical line, the following depths were chosen: 0, 0.1, 1.0, 1.5, 3.0, 3.5, 5.0, 7.5, 10.0, 12.5, 13.0, 14.5, 16.0, 17.5, 19.0, 20.5, 22.0, 23.5, 25.0, 26.5, and 28.0 m. In the fist stage, steady fields of currents and turbulence were computed for eight main directions of wind according to the model given in [51]. The wind velocity was assumed to be equal to 10 m/sec.

In the solution of the optimization problem, several additional requirements were imposed: the depth in the region of location of an oil terminal complex must be equal to at least 20 m and its distance from the shore must not exceed 15–20 miles. To satisfy these requirements, areas that do not meet these criteria were eliminated from consideration. Computations were carried out for eight wind situations for a period of $T = 7$ days. According to the evaluation made, for this period of time oil products reach the boundaries of the region for any location of a source.

A partial field of the quality functional J for the northwest type of atmospheric circulation and the resulting distribution obtained as a sample of the maximum among N values of the functional J at every point of the space are presented in Fig. 7.6. The latter can be used for making a decision concerning the location of an oil terminal complex because it reflects maximum possible values of the content of oil products in the water of nature-conservation areas for sources located at specific points of the domain Ω. The values of the functional are given in conventional units (c.u.) of the content corresponding to the source power $Q = 1$ c.u./sec. The problem reduces to the determination of extremum areas for the values of the functional. Computations showed that, on the whole, for different hydrometeorological situations these areas are locally stable but differ substantially in intensity. The area that best suits the requirements imposed on the location of an oil terminal complex is the area of the minimum of the functional with typical values less than 12 c.u. displayed in Fig. 7.6b. The location of an oil terminal complex in regions with maximum values of the functional J (the Zernov phyllophorous field (up to 500 c.u.), the region of Odessa sand bank (more than 150 c.u.), the beam of the Malyi Fontan Cape (more than 80 c.u.), and Kryzhanovka settlement (more than 70 c.u.)) is the most dangerous for the selected nature-conservation areas.

In addition to the problem described above, the model of self-purification was also used for the solution of the problem of prediction of the level and extent of pollution of the marine medium in the case of oil outflow with regard for the loss of oil due to evaporation (for a detailed description and results, see [53, 55, 141]).

7.3. Assessment of the Role of Coastal Anthropogenic Sources of Pollution in the Formation of Water Quality in the Odessa Region of the Northwest Part of the Black Sea

As indicated in Sec. 2.2.1, the water quality of the Odessa region of the northwest part of the Black Sea is determined, on the one hand, by the inflow of biogenic and polluting substances with the discharge of the Dnieper, Yuzhnyi Bug and, to a lesser extent, Dniester and, on the other hand, by the operation of anthropogenic pollution sources in the near-shore area of the Odessa megalopolis (Il'ichevsk–Odessa–Yuzhnyi).

Table 7.1. Relative Contribution of the Discharge of the Dnieper, Yuzhnyi Bug, and Dniester and the Combination of Anthropogenic Sources with Respect to the Mass of Supplied Biogenic Substances

Biogenic substance	Measure-ment unit	Anthropogenic source, Odessa	Dnieper	Yuzhnyi Bug	Dniester	Total
BOD_{tot}	ton/yr	1924.1	204353.3	10274.4	39366.4	255918.2
	%	0.75	79.85	4.02	15.38	100
NH_4^+	ton N/yr	353.8	8514.7	5194.0	2606.4	16669.0
	%	2.12	51.08	31.16	15.64	100
NO_3^-	ton N/yr	2401.7	8041.7	6925.3	1617.8	18986.5
	%	12.65	42.35	36.47	8.53	100
PO_4^{3-}	ton P/yr	681.7	11353.0	4512.8	1258.3	17805.7
	%	3.83	63.76	25.34	7.07	100

In the development of the strategy of preservation and improvement of water quality of this water area, an important role is played by the problem of the determination of the influence of river discharge and coastal anthropogenic sources on the existing level of trophity and pollution of waters.

The specific feature of the Odessa region of the northwest part of the Black Sea is its relative remoteness from the mouth areas of rivers, whereas coastal anthropogenic sources discharge polluted waters directly into the near-shore part of the water area.

The results of the evaluation of the contribution (with respect to the supplied mass of biogenic substances) of the river discharge and the combination of anthropogenic sources are given in Table 7.1. These results are true for the northwest part of the Black Sea as a whole, but they are not completely correct in the specific case of the water area of the Odessa region because the level of hydrodynamic dilution of river waters that reach the boundaries of this region and the level of waste waters of anthropogenic sources located directly on its shores are different. As a result, a considerable difference in the amounts of biogenic substances coming from these two main groups of sources can be compensated by different degrees of the hydrodynamic dilution of waters, which depend on the regional hydrological conditions and can be evaluated only with the use of the hydrodynamic part of the water-quality model.

The computational region (bounded by the coordinates 46°00′–47°37′ N and 30°24′–32°17′ E) is approximated by a space grid with 72×38 nodes with step 2000 m. The time step is equal to 6 sec for the barotropic component of the current velocity and 72 sec for the baroclinic component. Ten computational depths in the σ-system of coordinates were used. Computation was carried out with assimilation of the hydrometeorological data of 1981 and 1986 from the first decade of March to the end of August. The seasonal variability of the flow rate of the river discharge of the Dnieper, Yuzhnyi Bug, and Dniester was taken into account (see Sec. 3.4).

The concentration of biogenic substances in river waters used in the computation is given in Table 2.8. The characteristic of waste waters of coastal anthropogenic pollution sources of the Odessa region of the northwest part of the Black Sea is given in Table B.4 and in [104], and their location is shown in Fig. 2.13. The storm discharge, which is of sporadic nature, was not taken into account in computations.

The contribution, evaluated by using the hydrodynamic model [103], of coastal anthropogenic pollution sources, relative to the influence of the discharge of the Dnieper, Dniester, and Yuzhnyi Bug [105], to the maintenance of the present, fairly high, level of trophity of waters of the Odessa region is displayed in Figs. 7.7–7.9. The space distributions of the concentrations of biogenic substances were computed under the assumption of their conservative nature with and without regard for the discharge of coastal sources. For the evaluation of the relative contribution of these sources, the following formula was used:

$$\eta_{i,j} = \left(\frac{C_{i,j}^{r+a}}{C_{i,j}^{r}} - 1 \right) \cdot 100\%, \tag{7.10}$$

where $\eta_{i,j}$ is the percentage of the contribution of coastal anthropogenic sources of pollution to the total concentration of the biogenic substance in the marine medium, $C_{i,j}^{r+a}$ is the concentration of the biogenic substance at the node (i, j) of the computational grid with regard for the discharge of coastal sources and the river discharge, and $C_{i,j}^{r}$ is the concentration of the biogenic substance at the same node with regard for the river discharge only.

The results of computation show that, for the used scale of initial dilution of 4 km^2 (caused by the 2000 m step of the horizontal computational grid), the contribution of coastal sources to the formation of the concentrations of mineral compounds of the main biogenic elements at different points of the water area of the Odessa region varies (depending on the hydrometeorological conditions and the remoteness of the near-shore area) within the range of 1–15% for ammonia nitrogen, 5–60% for phosphate phosphorus, and 2–40% for nitrate nitrogen with respect to the total amount of these substances coming from external sources (Figs. 7.7–7.9).

The seasonal estimates for the contribution of coastal anthropogenic sources of pollution to the formation of concentrations of mineral compounds of biogenic elements and organic matter observed in the Dnieper–Bug region of the northwest part of Black Sea obtained with the use of the eutrophication model are presented in Figs. 7.10 and 7.11. We see that, in spring, for the horizontal step of the computational grid equal to 2000 m, the discharges of coastal sources provide an increase in the biomass of phytoplankton in the Odessa region from 3% (in the sea region) to 18% (in the near-shore area), the content of BOD_5 up to 8%, and the content of phosphates up to 30–60% with respect to the values of these characteristics determined by the interecosystem biochemical processes of transformation of substances and the influence of the discharge of the Dnieper and Yuzhnyi Bug (Fig. 7.10).

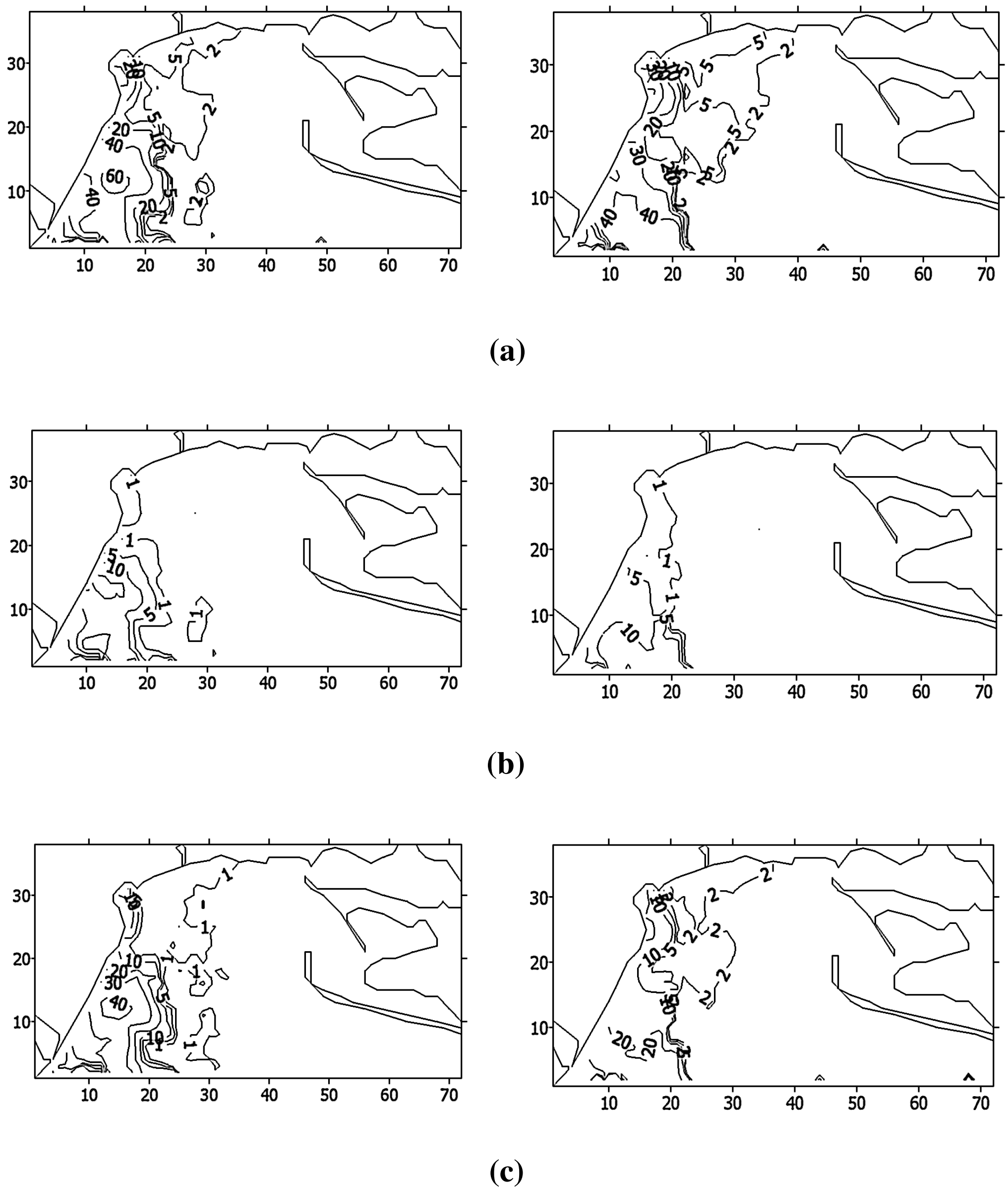
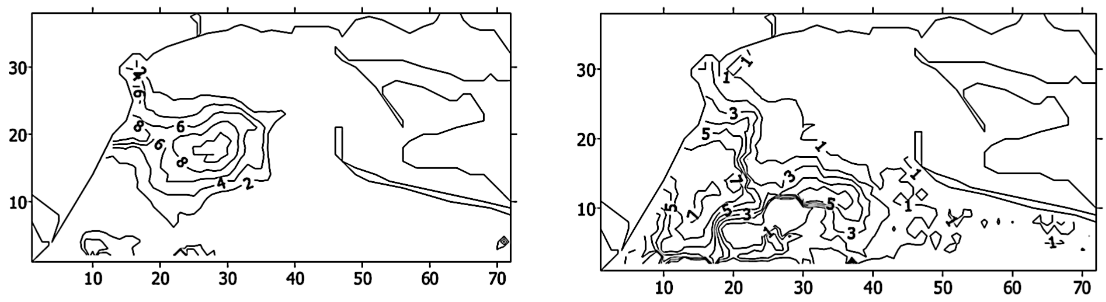
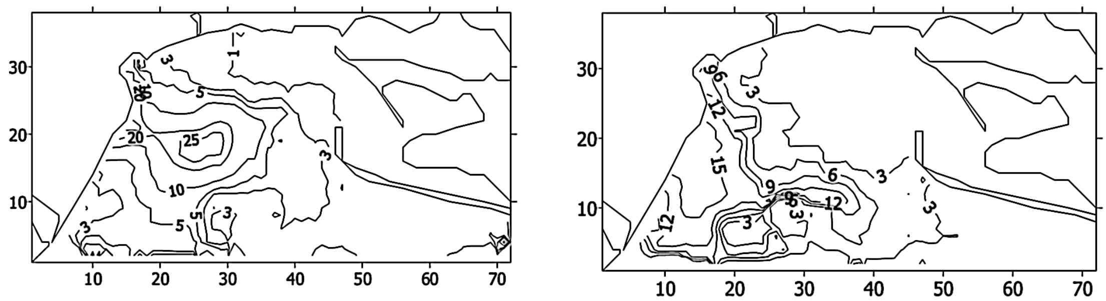


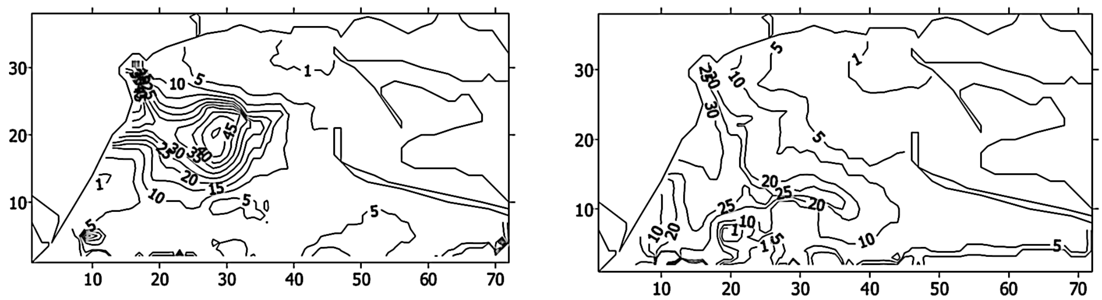
Fig. 7.7. Contribution (in %) of coastal anthropogenic sources of the Odessa region to the formation of the present-day level of the content of phosphate phosphorus (a), ammonia nitrogen (b), and nitrate nitrogen (c) in the photic layer of the northwest part of the Black Sea relative to the removal of these substances by river discharge computed on the basis of the hydrodynamic model for the middle (on the left) and the end (on the right) of April. Hydrometeorological conditions of 1986.



(a)



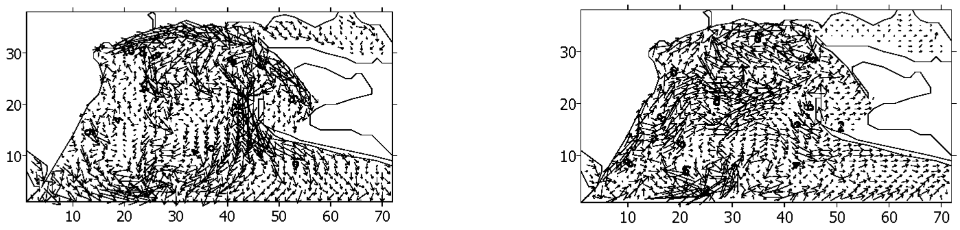
(b)



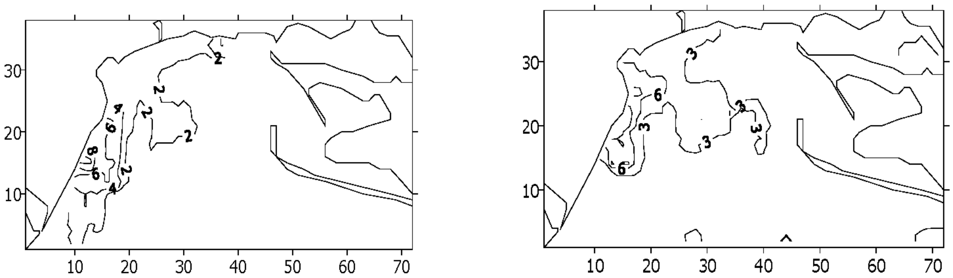
(c)

Fig. 7.8. Contribution (in %) of coastal anthropogenic sources of the Odessa region to the formation of the present-day level of the content of ammonia nitrogen (a), nitrates (b), and phosphate phosphorus (c) in the photic layer of the northwest part of the Black Sea at the end of April (on the left) and at the beginning of May (on the right) relative to the removal of these substances by river discharge under wind conditions of 1981.

The intensive inflow of phosphates with the waste waters of coastal sources leads to an increase in the rate of synthesis of organic matter and consumption of mineral nitrogen by phytoplankton. This leads to a decrease in the content of ammonia nitrogen and, to a lesser extent, nitrates in waters of the area. The contribution of coastal anthropogenic sources to the pollution of the marine system is maximum in the regions of discharge of waste waters of the "Severnaya" and "Yuzhnaya" stations of biological purification.



(a)



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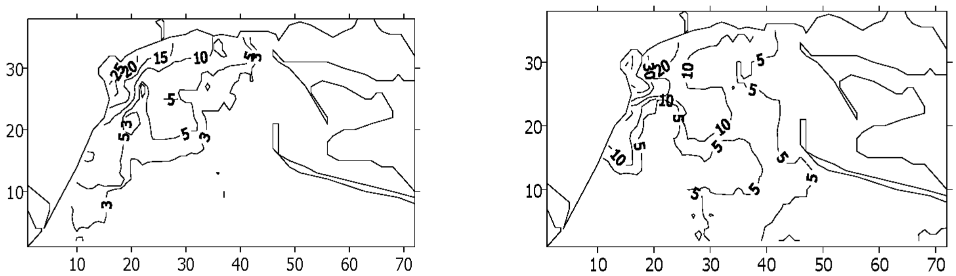
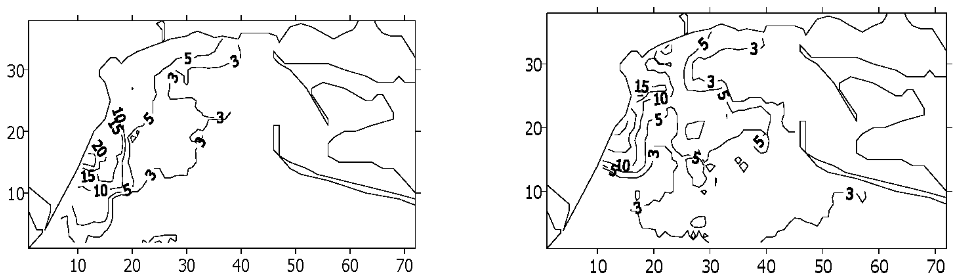


(c)



(d)

Fig. 7.9. Surface currents (a), cm/sec, and the contribution (in %) of coastal anthropogenic sources of the Odessa region to the formation of the present-day level of the content of ammonia nitrogen (b), nitrates (c), and phosphate phosphorus (d) in the photic layer of the northwest part of the Black Sea at the end of July (on the left) and at the end of August (on the right) relative to the removal of these substances by river discharge under hydrometeorological conditions of 1986.

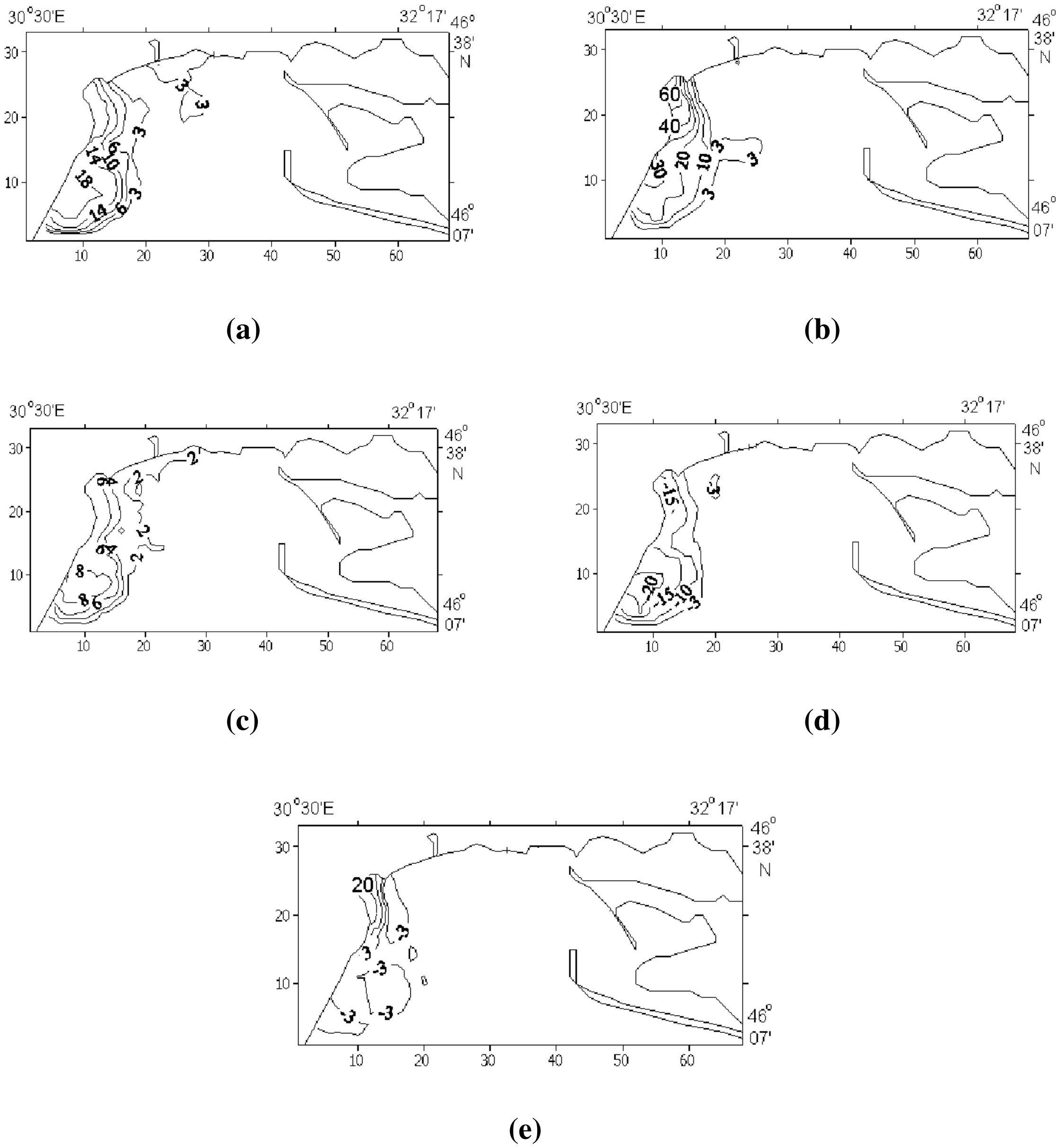


Fig. 7.10. Contribution (in %) of coastal anthropogenic sources of the Odessa region to the formation of the biomass of phytoplankton (a), the content of phosphate phosphorus (b), BOD_5 (c), ammonia nitrogen (d), and nitrate nitrogen (e) in the photic layer of the northwest part of the Black Sea computed on the basis of the eutrophication model for the end of April, 1986.

The contribution of coastal sources in a summer season is displayed in Fig. 7.11. Despite a decrease in river discharge, the direct contribution of coastal sources to the eutrophication of waters of the Odessa region considerably decreases as compared with the spring, which can be explained by the fact that the water temperature equal to 20–23° C in the photic layer in summer is optimal for processes of mineralization of organic matter. As a result, the inflow of mineral compounds of biogenic elements caused by these processes becomes comparable with the inflow caused by coastal anthropogenic pollution sources.

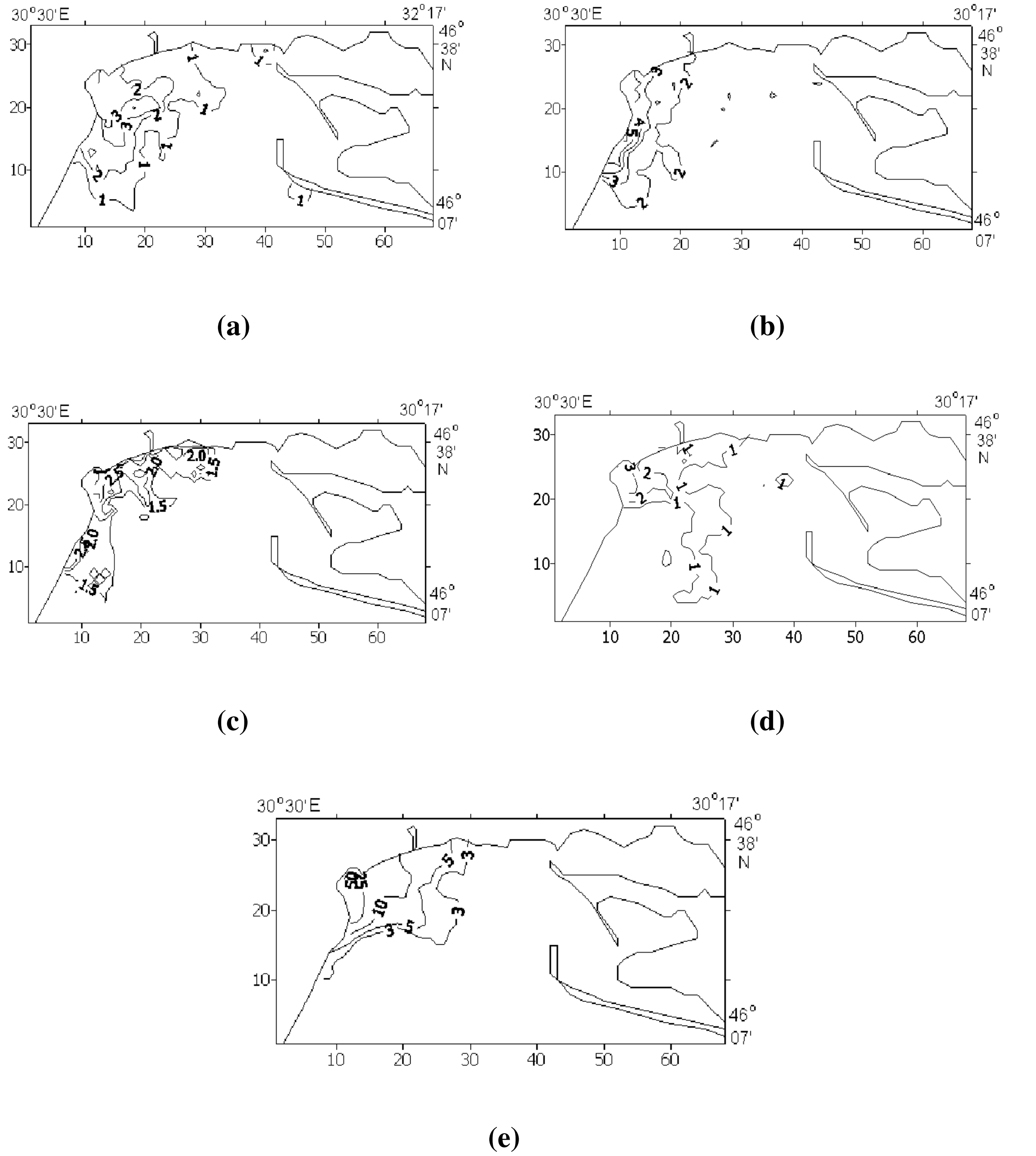
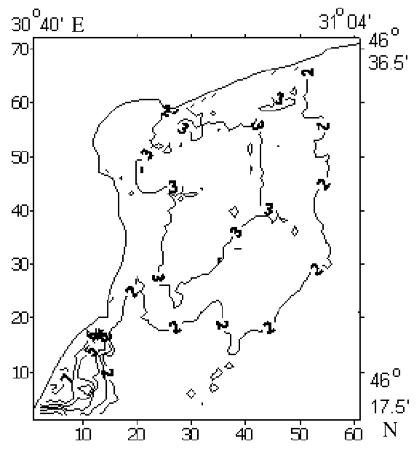
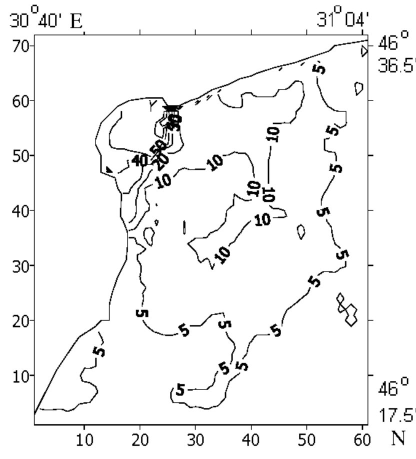


Fig. 7.11. The contribution, in %, of coastal anthropogenic sources of the Odessa region to the formation of the biomass of phytoplankton (a), the content of phosphorus of phosphates (b), BOD_5 (c), ammonia (d) and nitrate (e) nitrogen in the photic layer of the northwest part of the Black Sea computed on the basis of the model of eutrophication for the middle of August of 1986.

The estimates for contributions described above were obtained for the scale of the initial dilution of waste waters of 4 km^2, and, hence, they are true if the Odessa region is considered as a whole as the large water area of the northwest part of the Black Sea bounded by the beams of the Sukhoi and Adzhalyksii firths. For the near-shore area of the sea, it is obvious that the contribution of pollution sources to the formation of water quality increases as these sources are approached.



(a)



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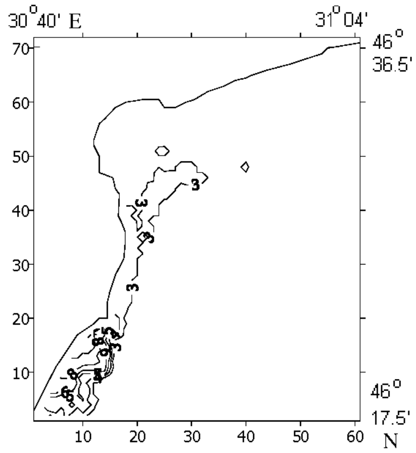
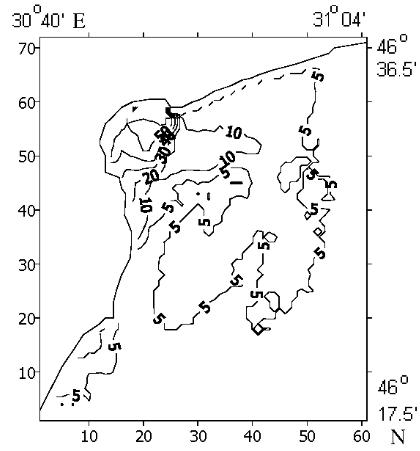


(c)



(d)

Fig. 7.12. Contribution (in %) of coastal anthropogenic sources of pollution to the formation of the biomass of phytoplankton ((a) and (b)) and the content of BOD_5 ((c) and (d)) in the photic layer of the Odessa region of the northwest part of the Black Sea in the absence ((a) and (c)) and presence ((b) and (d)) of discharge of the "Severnaya" station of biological purification computed on the basis of the eutrophication model for mid August of 1986.

The estimates for the contribution of coastal anthropogenic sources to the eutrophication of waters of the Odessa region of the northwest part of the Black Sea presented in Figs. 7.12–7.13 were obtained with the use of the eutrophication model and relation (7.10) for the scale of the initial dilution of 0.25 km^2 (computational grid with horizontal step 500 m). Computations were performed only for the water area of the Odessa region (see Fig. 2.1) covered with a horizontal computational grid with 61 × 72 nodes with space step 500 m. Ten calculated levels along the vertical coordinate were used. Computations were carried out for 30 days of model time under hydrometeorological conditions of August,

1986. The initial distribution of modeled characteristics with respect to depth and their variability at the marine boundaries of the water area were specified on the basis of the results of computation for the entire Dnieper–Bug near-mouth region of the northwest part of the Black Sea. The distribution of characteristics in the horizontal planes was assumed to be uniform. To decrease the influence of the boundary conditions on the obtained results, computations were performed for a fixed space thermal structure of waters, whereas the other modeled variables, including salinity, were computed in the prognostic mode.

One of the strongest (in the quantitative sense) coastal anthropogenic sources of pollution of waters of the Odessa region of the northwest part of the Black Sea is the "Severnaya" station of biological purification (see Tables 2.7 and B.4). This station does not have an equipment for deep-water discharge of waste waters, and the discharge is performed at a distance of 300 m from the shore into a shallow near-shore area. For this reason, the regulations for its operation in the mode of minimization of ecological risk assume the discharge of waste waters in May–mid-September not into the sea but into the Khadzhibei Firth. Exactly this mode of operation of the "Severnaya" station of biological purification was considered in the previous computations. However, in several recent years, due to the maximum critical levels of water reached in the Khadzhibei Firth, waste waters of the "Severnaya" station of biological purification have been discharged into the shallow near-shore area of the sea all over the year. For this reason, the evaluation of the contribution of coastal anthropogenic sources to the formation of the level of trophity of waters of the Odessa region in the summer period was performed for two cases corresponding to the presence and the absence of discharge of the "Severnaya" station of biological purification into the sea.

Computations showed (see Figs. 7.12–7.13) that, as could be expected, if the scale of the initial dilution of waste waters is decreased to 0.25 km^2 and the near-shore area of the sea is considered with horizontal space step 500 m, then the role of anthropogenic sources in the formation of concentrations of mineral compounds of biogenic elements and organic matter increases. In the absence of discharge of the "Severnaya" station of biological purification, the maximum values of estimates for an increase in the biomass of phytoplankton (> 7%), BOD_5 (> 8%), and phosphates (75%) are obtained in the near-shore area in the region of location of the "Yuzhnaya" station of biological purification. A considerable increase in the concentration of nitrates (up to 40%) occurs due to the inflow of drainage waters. The content of ammonia nitrogen changes insignificantly (up to 3%) because it is actively assimilated by phytoplankton in the course of intensification of photosynthesis caused by the additional inflow of phosphates from coastal anthropogenic sources. As a result, the role of a biogenic element that restricts the production of phytoplankton passes from mineral phosphorus to mineral nitrogen.

In the case of discharge of waste waters from the "Severnaya" station of biological purification to the near-shore area in the summer period, they become an important source of eutrophication of the marine medium of the Odessa region. The concentration of phosphates and nitrates in the Odessa Bay increases by a factor of three to five, and the biomass of phytoplankton and the value of BOD_5 increase by 50% (Figs. 7.12 and 7.13). For the reasons indicated above, the content of ammonia nitrogen decreases by 2–5% in most part of the water area.

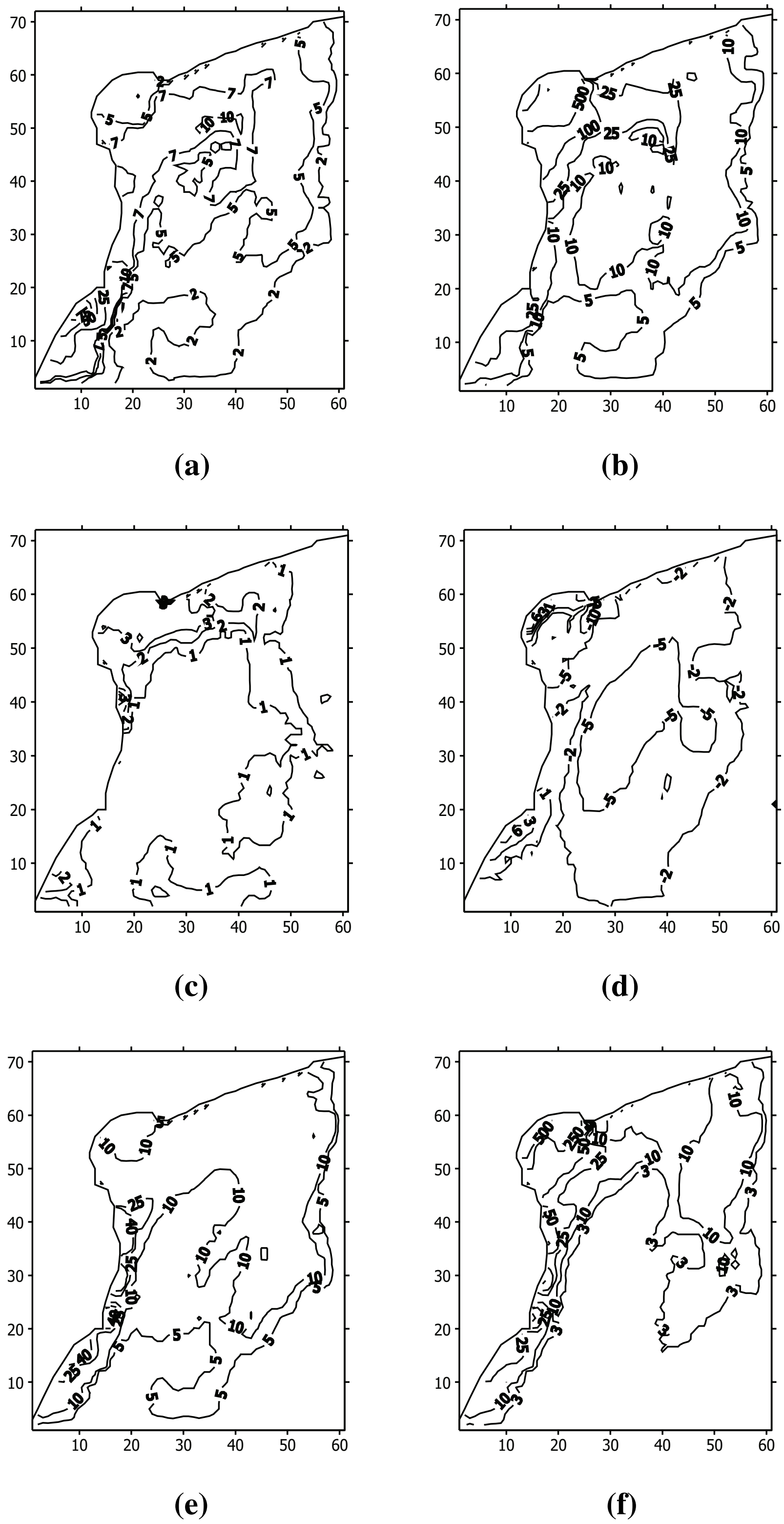


Fig. 7.13. Contribution (in %) of coastal anthropogenic sources of pollution to the formation of phosphate phosphorus ((a) and (b)), ammonia nitrogen ((c) and (d)), and nitrates ((e) and (f)) in the photic layer of the Odessa region of the northwest part of the Black Sea in the absence ((a), (c), (e)) and presence ((b), (d), (f)) of discharge of the "Severnaya" station of biological purification computed on the basis of the eutrophication model for mid August of 1986.

Thus, it follows from the presented results of computations that, with regard for the different degrees of hydrodynamic dilution of river and waste waters, the contribution of the latter to the formation of the concentrations of biogenic substances observed in the Odessa region of the northwest part of the Black Sea, under the assumption of their conservativeness and for the discretization of the water area with horizontal space step 2 km, does not exceed 8–15% for ammonia nitrogen, 25–40% for nitrate nitrogen, and 20–60% for phosphate phosphorus, depending on a season and hydrometeorological conditions (wind, flow rates of rivers, etc.).

The results obtained by using the eutrophication model show that, in the spring period, the operation of coastal anthropogenic pollution sources leads to an increase in the biomass of phytoplankton by 3–20%, the value of BOD_5 by 2–9%, and the content of phosphates to 60%. The intensive inflow of phosphates with waste waters of coastal sources leads to an increase in the production of phytoplankton and, as a result, a decrease in the concentration of mineral nitrogen in waters of the water area.

In the summer period, the interecosystem processes of regeneration of inorganic compounds of biogenic elements become more intensive in the course of mineralization of organic matter. The duration of biochemical cycles of biogenic elements decreases. In the optimal mode of operation, the discharge of waste waters from the "Severnaya" station of biological purification to the sea terminates in summer. The seasonal pycnocline becomes more intensive, which hampers the inflow of waste waters from the deep region of discharge to the photic layer. As a result, the role of coastal anthropogenic sources as a source of biogenic elements and a stimulator of the process of primary production of organic matter substantially decreases. In particular, the increment in the biomass of phytoplankton caused by the discharge of coastal sources decreases to 3%, the concentration of phosphates to 5%, the concentration of ammonia to 3%, and BOD_5 to 2.5%.

For the space resolution of 500 m, the contribution of coastal anthropogenic sources to the formation of the concentration of phosphates observed in the summer period in the near-shore area increases to 75%, the concentration of phytoplankton to 7%, and BOD_5 to 8%.

The ecological situation in the Odessa region of the northwest part of the Black Sea, and especially in the Odessa Bay, substantially deteriorates in the case of discharge of waste waters from the "Severnaya" station of biological purification into the sea in summer. In this case, the biomass of phytoplankton and BOD_5 in waters of the Odessa Bay increase by 50% and the content of phosphates and nitrates increases by a factor of two to five.

Generalizing the obtained results, one should note that the operation of coastal anthropogenic sources does not dominate the ecological situation in the open marine water area of the Odessa region of the northwest part of the Black Sea. However, within the limits of the two-mile nature-conservation near-shore area [89], their influence on seawater quality is significant. It should be expected that the maximum effect can be achieved by the regulation of the discharge of biogenic substances of coastal sources in the spring period. Furthermore, it is preferable to decrease the discharge of pollutants containing phosphorus as a biogenic element that restricts the primary production of organic matter by phytoplankton. The discharge of waste waters by the "Severnaya" station of biological purification into the sea in summer leads to the domination of this source in the eutrophication of waters of the Odessa Bay and a considerable increase in the eutrophication of waters of the water area on the whole. In the case of the operation of the "Severnaya" station of biological purification in summer in the recommended mode of discharge of waste waters into the Khadzhibei Firth, the contribution of the other coastal anthropogenic sources to the eutrophication of waters of the marine part of the water area of the Odessa region does not exceed several percents, i.e., their discharge, in fact, does not have any effect on the development of the ecological situation.

The presented values of estimates for the contribution of coastal anthropogenic sources to the formation of the level of trophity of waters of the Odessa region of the northwest part of the Black Sea illustrate how regional nature-conservation procedures can improve the present-day ecological situation in this water area on the whole and in its near-shore part in particular. For a more radical improvement, procedures aimed at an increase in the quality of river waters should be realized at the national level.

In addition to biogenic substances, the river discharge also brings toxic pollutants into the water area of the northwest part of the Black Sea. Their propagation in the marine medium is described by the model of self-purification of water. The evaluation of the possible background level of the content of pollutants formed in the water area of the Odessa region by the discharge of the Dnieper and Yuzhnyi Bug is of undoubted interest.

The results of computations on the basis of the model of self-purification for dissolved pollutants with different resistance to processes of physicochemical and biochemical destruction are presented in Fig. 7.14. As the source of pollution, the discharge of the Dnieper and Yuzhnyi Bug in the spring period was considered. The concentration of pollutants in river waters was assumed to be equal to 100 conventional units (percents). The background concentrations of pollutants at the initial time and at the open sea boundary was assumed to be equal to 10^{-12} c.u. Computations were carried out under the meteorological conditions of 1986 on March 10–May 20, when the fresh-water discharge of the Dnieper-Bug Firth attains its maximum values.

The obtained results characterize the rate of decrease in the concentrations of pollutants of various types as the distance from the sources increases and the expected level and scales of pollution of the investigated water area. According to the results of computations, the concentrations of pollutants resistant to the biochemical destruction (with integral coefficients of destruction K_{ci} within the range 0.005–0.05 day^{-1}) that arrive with the discharge of the Dnieper and Yuzhnyi Bug in the surface layer of waters of the Odessa region are equal, in the mean, to 3–20% of the original values in the sources. Pollutants of this type are, e.g., DDT, synthetic surface-active substances, and stable fractions of oil products [83, 84]. In the waters of the Odessa region, the concentrations of biologically "soft" pollutants (e.g., phenols and colon bacillus) with coefficients of destruction equal to 0.1 day^{-1} and higher are equal to 1% and lesser of their content in river waters. As K_{ci} increases to 0.5 day^{-1}, the region of pollution is localized near the mouths of rivers in the firth.

In Fig. 7.15, we present the results of computations carried out by using the model of self-purification of waters for a specific type of pollutant, namely, the emulsified and dissolved part of oil products, whose rate of destruction in the spring temperature range was assumed to be equal to 0.03 day^{-1} [82, 84] and whose concentration in river waters, according to data of field observations of the Odessa Branch of the Institute of Biology of Southern Seas for 1995, was equal to 0.7 mg/liter for the Yuzhnyi Bug and 0.13 mg/liter for the Dnieper. These computations show that, as a result of the inflow of oil products with river discharge, background concentrations of this pollutant of order 5–10 μg/liter, which amounts to 10–20% of the maximum allowable concentration, are formed in the Odessa region of the northwest part of the Black Sea.

As indicated in Sec. 2.2.1, among strong coastal pollution sources of the Odessa near-shore area there are storm discharges, whose specific features are sporadicity and intensity. In the summer period, sanitary-epidemiological services periodically prohibit the use of seawater at many town beaches, which, in most cases, is connected with the inflow of storm waters from the territory of the town via the main storm discharge outlets.

According to [117], the hydrochemical and microbiological characteristics of storm waters are identical to those of insufficiently purified and unpurified waste waters of industrial plants and municipal sewage collectors. In particular, they are characterized by high concentrations of oil products (≈ 24 mg/liter) and pathogenic microorganisms (coli index ≈ 1.285 millions of cells/liter), which are several orders of magnitude higher than the maximum allowable concentrations established for them in the near-shore sea water.

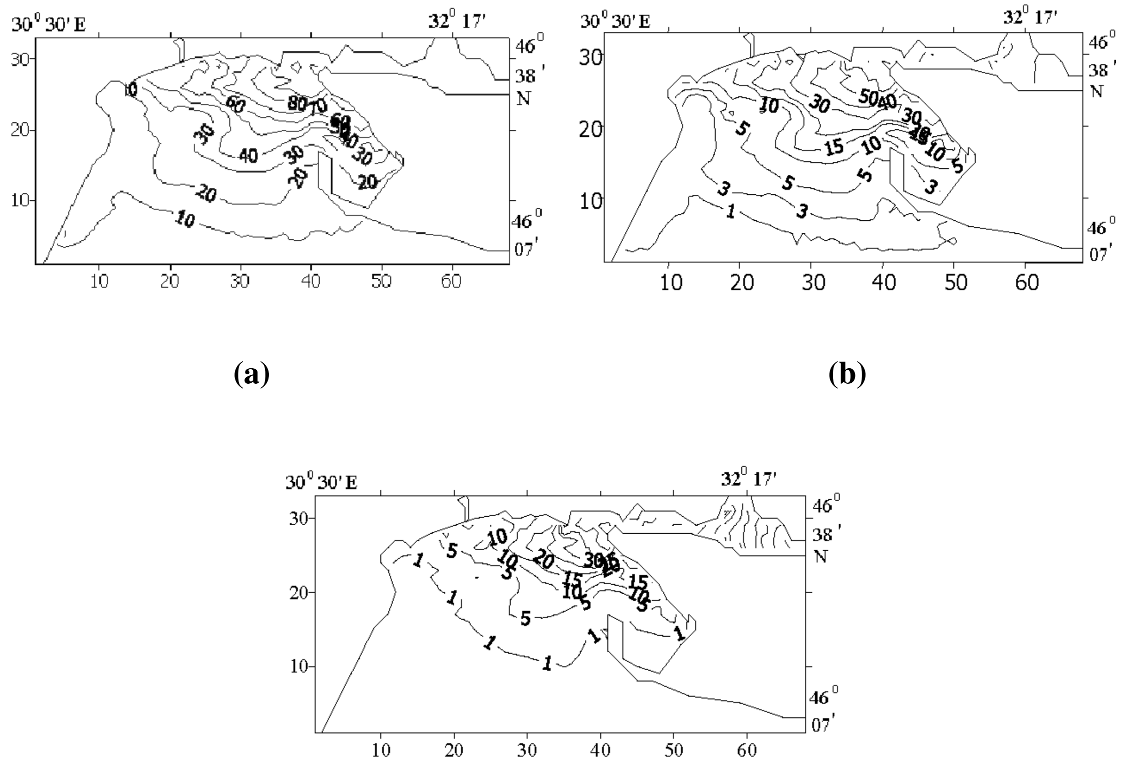
To calculate the damage to the marine medium caused by storm discharges in the period of intensive precipitation in the summer season of a year and to develop a plan of measures for the minimization of this damage, it is necessary to evaluate the level and space–time scales of pollution of the near-shore recreation sea area by storm discharges. This problem was solved by using the model of self-purification of seawater.

Model computations were carried out for two types of pollutants: oil products and microorganisms of the group of colon bacillus, whose concentration in storm-discharge waters is the highest as compared with the maximum allowable concentration. The considered water area (46°22.4′–46°33.6′ N, 30°44.6′–30°50.8′ E), which includes the region of Odessa coast from station 16 of Bol'shoi Fontan to Kryzhanovka, was covered by a grid of 31 × 80 nodes with horizontal space step 250 m. Nine computation depths were used. The flow rates of storm discharge were determined according to [107] for the heavy shower of July 10, 2004, which lasted for 3 h 25 min and resulted in a rainfall of 15.3 mm. Note that, on the average, a typical year in Odessa is characterized by 14 days with rainfall of 10 mm/day and 4 days with rainfall of 20 mm/day [21].

To take into account the influence of a seasonal pycnocline on the vertical diffusion of pollutants, the vertical distribution of water temperature typical of a summer period was specified in computations.

The coefficient of nonconservativeness for oil products was determined from the experimental data [82] on the dependence of the half-life of dissolved forms of oil τ_{nf}, in hours, on the water temperature T_w, in °C:

$$\tau_{nf} = 1260.42 - 54.928 T_w + 0.5688 T_w^2.$$



(a) **(b)**

(c)

Fig. 7.14. Distribution of pollutants of neutral buoyancy arriving with the discharge of the Dnieper and Yuzhnyi Bug and characterized by different values of the coefficient of nonconservativeness: $K_c = 0.005$ day^{-1} (a), $K_c = 0.05$ day^{-1} (b), $K_c = 0.1$ day^{-1} (c). Fields correspond to mid May under the meteorological conditions of 1986.

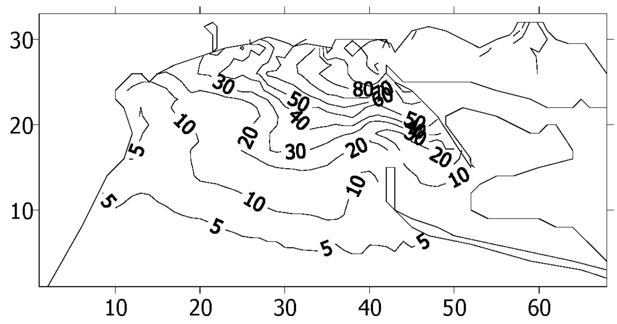


Fig. 7.15. Distribution of oil products, in μg/liter, arriving with the discharge of the Dnieper and Yuzhnyi Bug in mid May under the meteorological conditions of 1986 computed on the basis of the model of self-purification of waters.

The specific rate of biodegradation of microorganisms of the group of colon bacillus was determined by relation (4.4) without regard for the influence of illuminance.

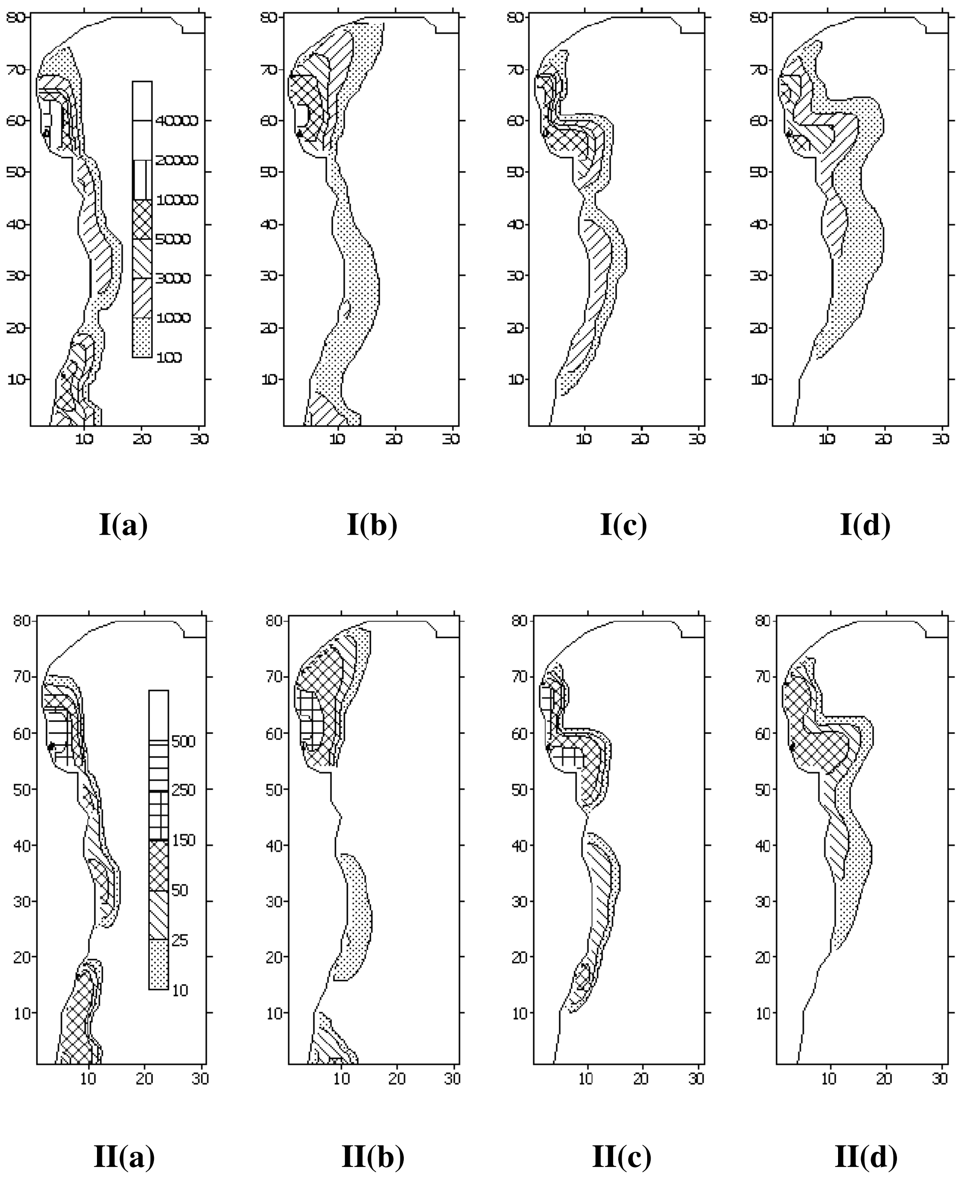


Fig. 7.16. Excesses of the background concentrations of coli index, in cell/liter, (I) and oil products, in μg/liter, (II) 15 h after the beginning (and ≈ 12 h after the end) ((a), (c)) and ≈ 24 h after the end ((b), (d)) of the discharge of storm waters to the near-shore area of the sea computed by using the model of self-purification for northwest ((a), (b)) and southeast winds with velocity of 5 m/sec.

The obtained results show that the storm discharge considerably deteriorates the seawater quality in the Odessa near-shore recreation area (Fig. 7.16). On the first day after precipitation, the coli index and the concentration of oil products exceed the maximum allowable concentration at the most part of the coast even without regard for the background level of pollution. However, due to the high rate of destruction of pollutants in the summer period of a year and the short time of discharge of storm waters, the level of pollution in near-shore waters decreases to the background values in two to three days after intensive precipitation.

7.4. Evaluation of the Efficiency of Nature-Conservation Engineering Measures Aimed at the Improvement of Water Quality in the Ciénaga de Tesca Lagoon

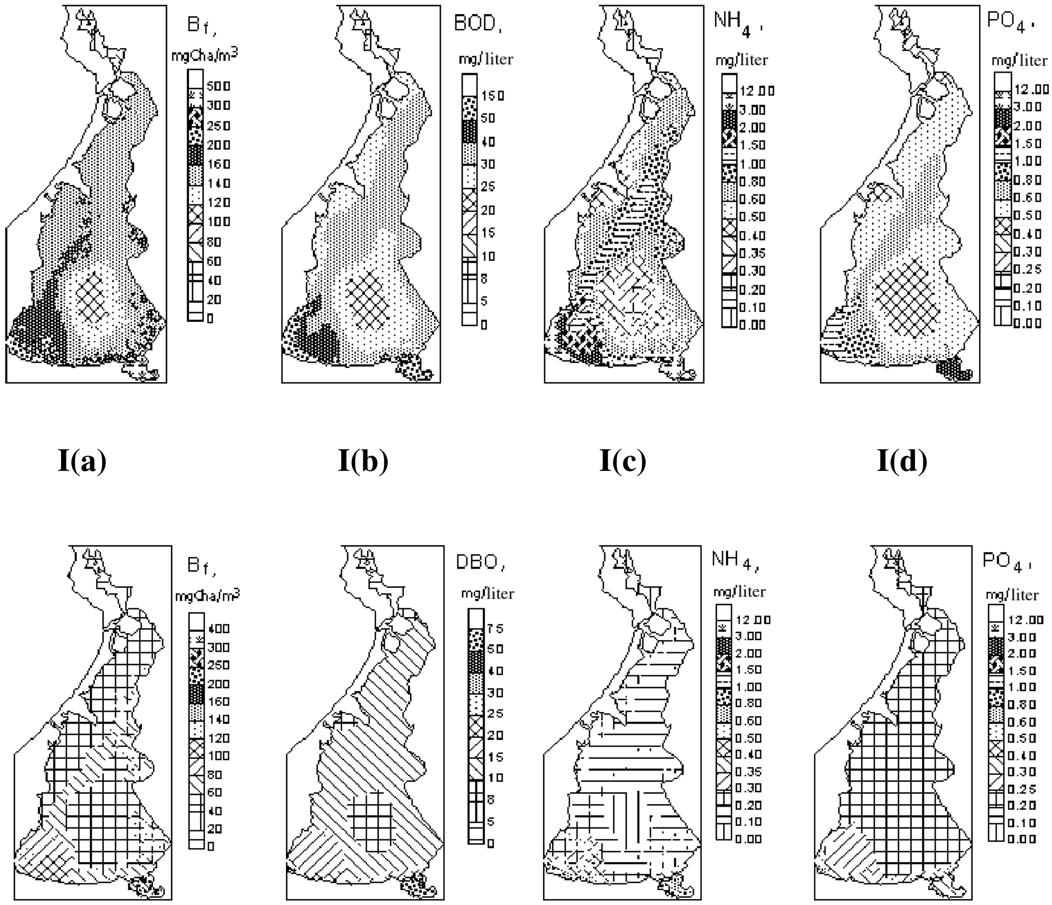
On the basis of a two-dimensional version of the model, the level of pollution of waters of the Ciénaga de Tesca lagoon in 2025 was predicted. This prediction was based on the assessment made in [133], according to which the discharge of waste waters to the basin will increase up to 95 350 m^3/day in agreement with the predicted growth of population of Cartagena. Only the flow rates of pollution sources were changed. It was assumed that the content of pollutants in waste waters remains the same. The flow rates of the sources for which prognostic information was absent were set equal to their present-day values. Computations were carried out under the conditions of the dry season of a year, for which the level of pollution in the southern part of the basin is maximum.

The results of numerical experiments with eutrophication model showed that, without active nature-conservation measures, the ecological situation in Ciénaga de Tesca in 2025 will considerably deteriorate as a result of an increase in the level of trophity and saprobity of its waters. For example, for the prognostic period the biomass of phytoplankton will increase from 110–130 to 150–200 mgChlA/m^3, the concentration of inert organic matter from 20–25 to 30–40 mgO_2/liter, the concentration of ammonia nitrogen from 0.4–0.6 to 0.8–1.5 mgN/liter, and the concentration of phosphates from 0.3–0.5 to 0.5–0.8 mgP/liter.

To avoid this scenario, it is planned to build a centralized sewer system of the town with outlet to the open sea [130]. This sewer system will remove 80% of household sewage of the town. The remaining 20% fall on the poor part of the town adjacent to the south boundary of the Ciénaga de Tesca lagoon, which will not be covered by the sewer system will be absent and whose polluted sewage will be discharged, as before, into the lagoon. The following question arises: “To what extent will the removal of 80% of the sewage predicted in 2025 improve the ecological situation in the lagoon?” An answer to this question was obtained by using the mathematical water-quality model [56, 144].

It was assumed that the centralized sewer system does not include sources 8 and 9 (see Table B.3 and Fig. 2.7), whose total flow rate is equal to ≈ 20% of the predicted total discharge of polluted waters in 2025.

Computations showed (Fig. 7.17.II) that the removal of 80% of the predicted discharge of polluted waters in 2025 considerably improves water quality in the lagoon as compared with both its predicted state (Fig. 7.17.I) and its present-day state (Fig. 5.14). The biomass of phytoplankton decreases to 50–60 mg ChlA/m^3, the content of inert organic matter to 10–12 mgO_2/liter, the content of ammonia nitrogen to 0.1–0.2 mgN/liter, and the content of phosphate phosphorus to 0.2–0.3 mgP/liter. However, as compared with the adjacent marine water area and according to the classification of [62], the water quality of the lagoon with respect to the content of phosphates, inert organic matter, and the biomass of phytoplankton still remains low, and the level of their trophity and saprobity remains high. The high level of pollution of waters in the south and southwest parts of the water area will persist.



I(a) **I(b)** **I(c)** **I(d)**

II(a) **II(b)** **II(c)** **II(d)**

Fig. 7.17. Space distribution of the biomass of phytoplankton, in mg ChlA/m^3, (a), inert organic matter, in mg O_2/liter, (b) ammonia, in mg N/liter, (c), and phosphates, in mg P/liter, (d) obtained on the basis of the model for conditions of a dry season of 2025 without (I) and with (II) removal of 80% of waste waters.

Another method for the improvement of water quality in the Ciénaga de Tesca lagoon was proposed by the Holland Engineering Company Haskoning [123]. This method is based on the intensification of hydrodynamic washing of the basin by the relatively clear sea water due to the construction of a system of waterworks including a channel located in the central part of the lagoon that connects the sea and a jetty, is directed from the north to the south, and divides the central and the south parts of the water area of the Ciénaga de Tesca lagoon into the east and the west parts (Figs. 7.18–7.19).

The efficiency of different ideas of the construction of a jetty and connecting channel was evaluated by using the water quality model. The following cases were considered:

(1) a channel 200 m wide and 1 m deep with uncontrolled mode of operation. A jetty is directed along the meridian and originates from the cape that separates the north and the central parts of the water area of the basin (Fig. 7.18.I).

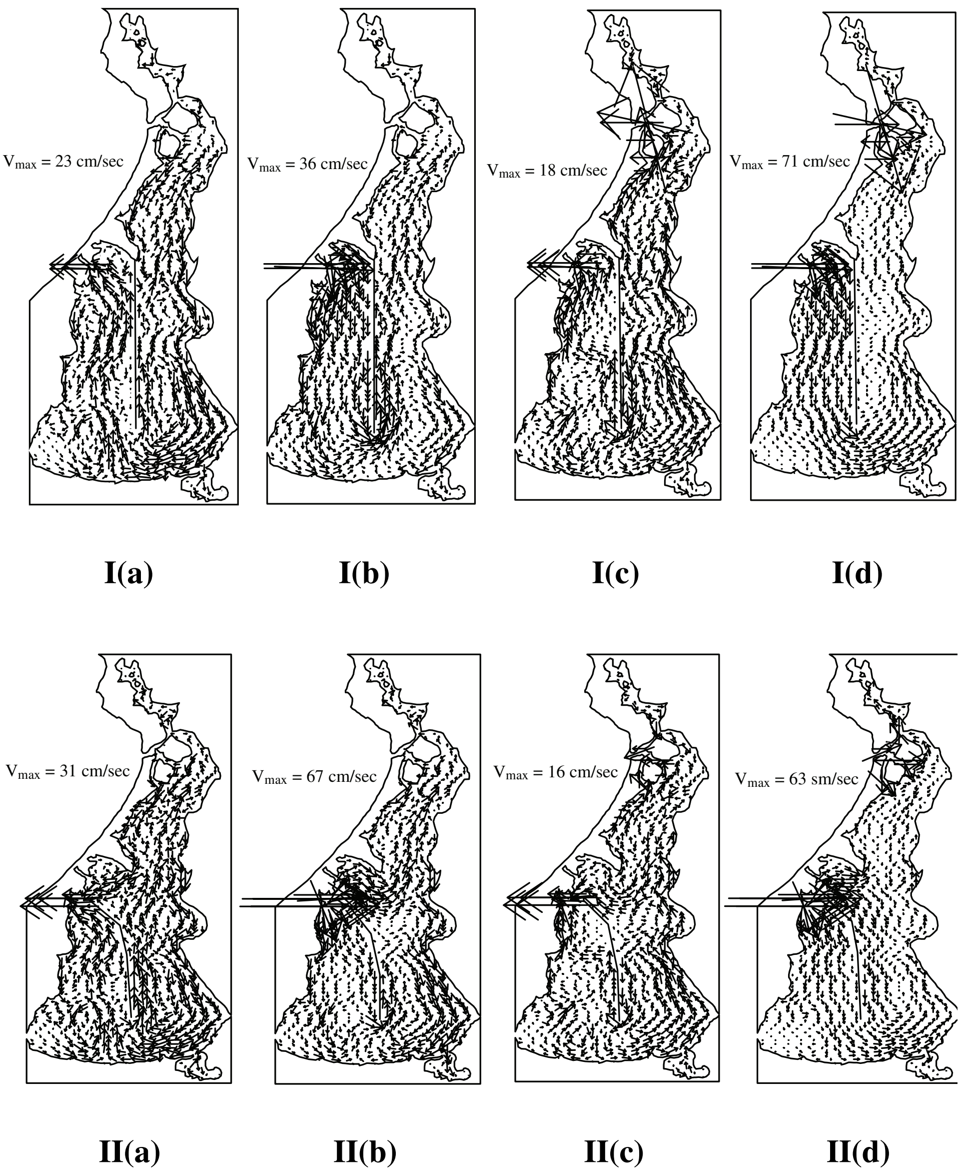


Fig. 7.18. Circulation of waters in the Ciénaga de Tesca lagoon in dry (low tide (a) and high tide (b)) and humid (low tide (c) and high tide (d)) seasons of a year for cases 1 (I) and 2 (II) of the construction of the jetty and the mode of operation of connecting channels.

(2) two channels 100 m wide and 1 m deep. A jetty is directed along the meridian and its origin is located between the channels. The south and the north channels connect the sea with the west and the east, respectively, parts of the basin. The mode of operation of the channels is uncontrolled (Fig. 7.18.II).

(3) the same as case 2 but with controlled mode of operation of channels. The south channel (lock) opens if the the sea-level checkmark is higher than the water-level checkmark in the basin (high tide). Conversely, the north channel opens if the sea-level checkmark is lower than the water-level checkmark in the basin (low tide) (Fig. 7.19).

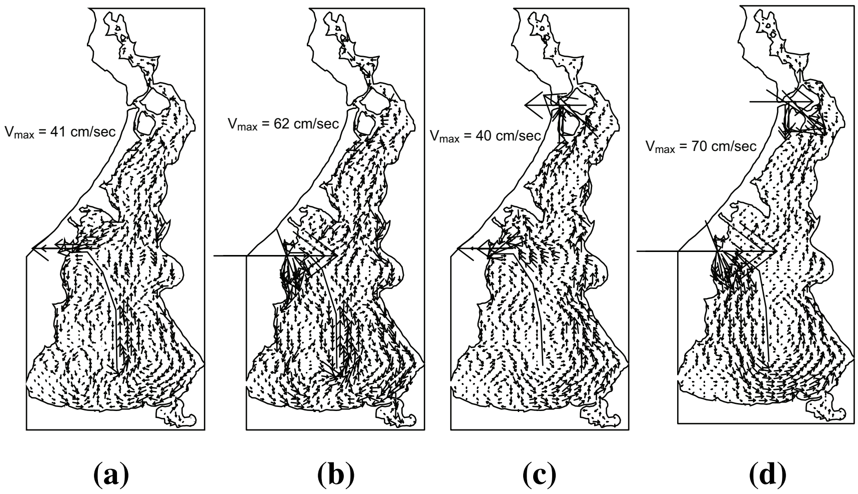


Fig. 7.19. Circulation of waters in the Ciénaga de Tesca lagoon in dry (low tide (a) and high tide (b)) and humid (low tide (c) and high tide (d)) seasons of a year for case 3 of the construction of the jetty and the mode of operation of connecting channels.

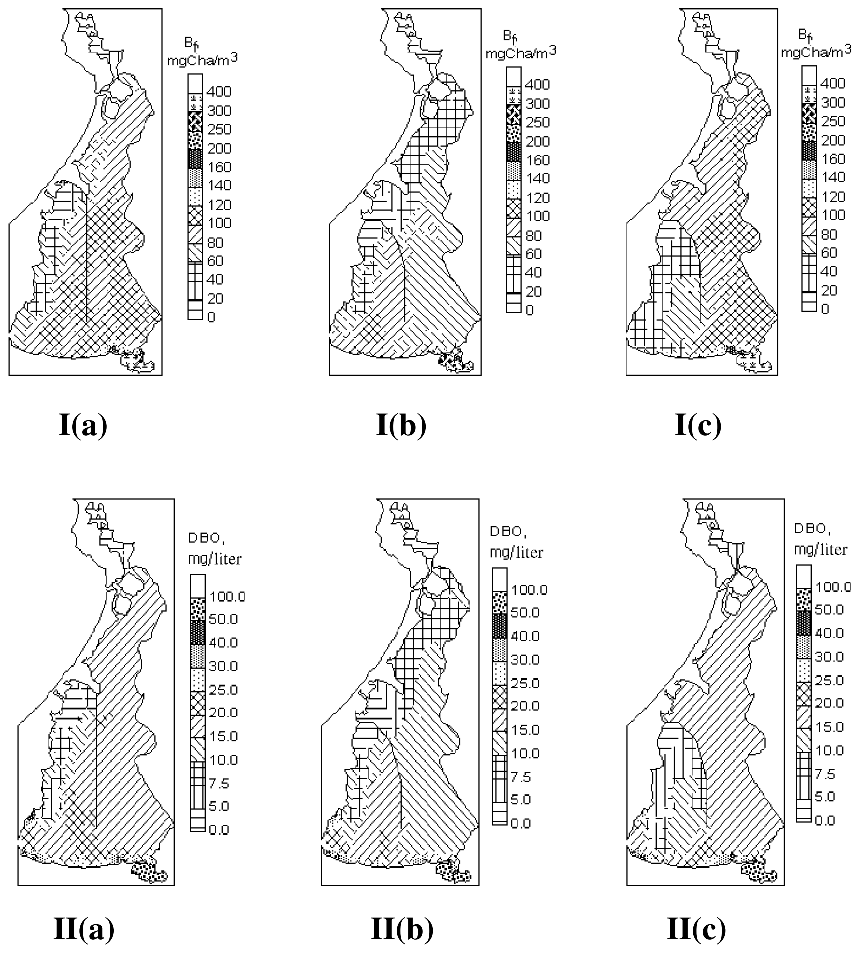


Fig. 7.20. Space distribution of the biomass of phytoplankton (I), in mg ChlA/ m^3, and the concentration of inert organic matter (II), in mg O_2/liter, determined on the basis of the model *for conditions of a dry season and present-day characteristics of the discharge* of waste waters in the case of the construction of waterworks: cases 1 (a), 2 (b), and 3 (c).

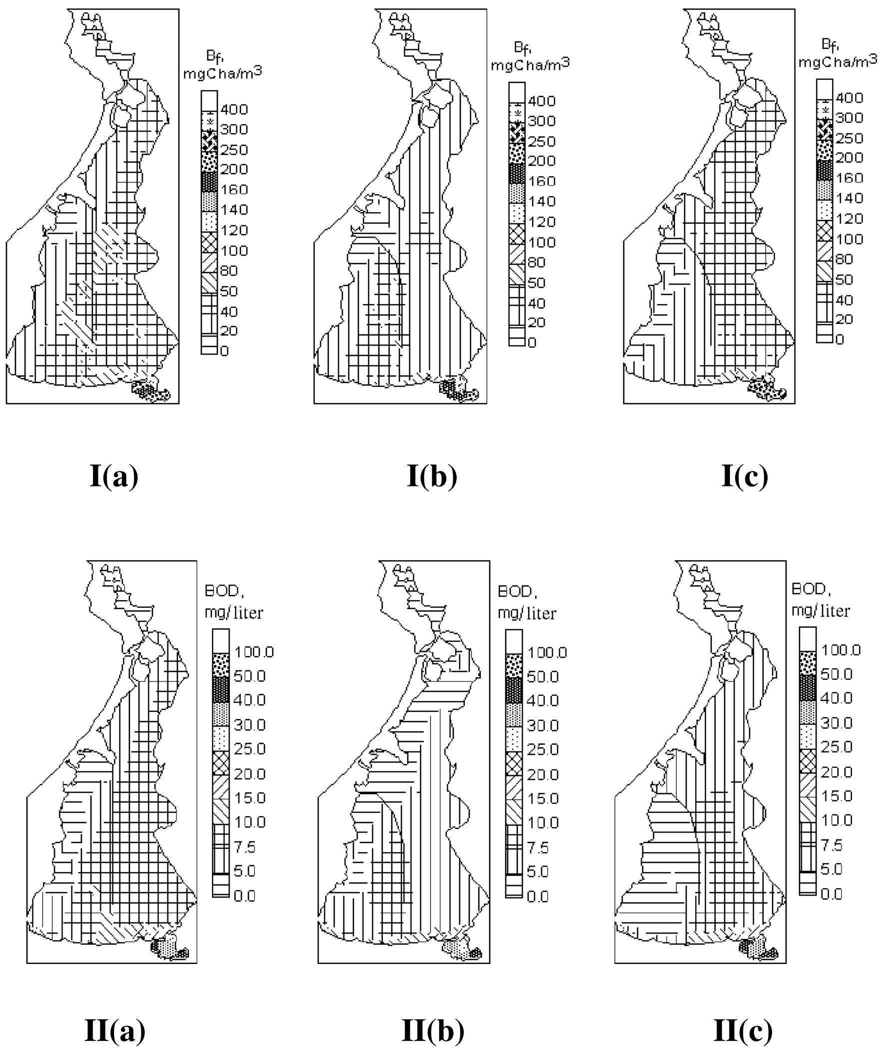


Fig. 7.21. Space distribution of the biomass of phytoplankton (I), in mg ChlA/ m^3, and the concentration of inert organic matter (II), in mg O_2/liter, determined on the basis of the model *for conditions of the dry season of 2025 in the case of the removal of 80% of discharge* and the construction of waterworks: cases 1 (a), 2 (b), and 3 (c).

It follows from Figs. 7.18–7.19 that the construction of channels and a jetty essentially changes the system of circulation of waters in the lagoon. The structure of currents and water exchange between the east and west parts of the water area separated by a jetty varies in a complicated manner during a day in accordance with day oscillations of the wind velocity and tidal oscillations of the sea level at the marine boundary.

The results of computation of the space distribution of some most informative parameters of water quality of the lagoon obtained in the case of realization of the engineering alternatives indicated above with preservation of the present-day values of discharge of pollutants are displayed in Fig. 7.20. One can see that the construction of waterworks improves the ecological situation in the Ciénaga de Tesca lagoon, but not radically, and, hence, it cannot be regarded as an alternative of the removal of 80% of the discharge of sources due to the construction of an integrated sewer system.

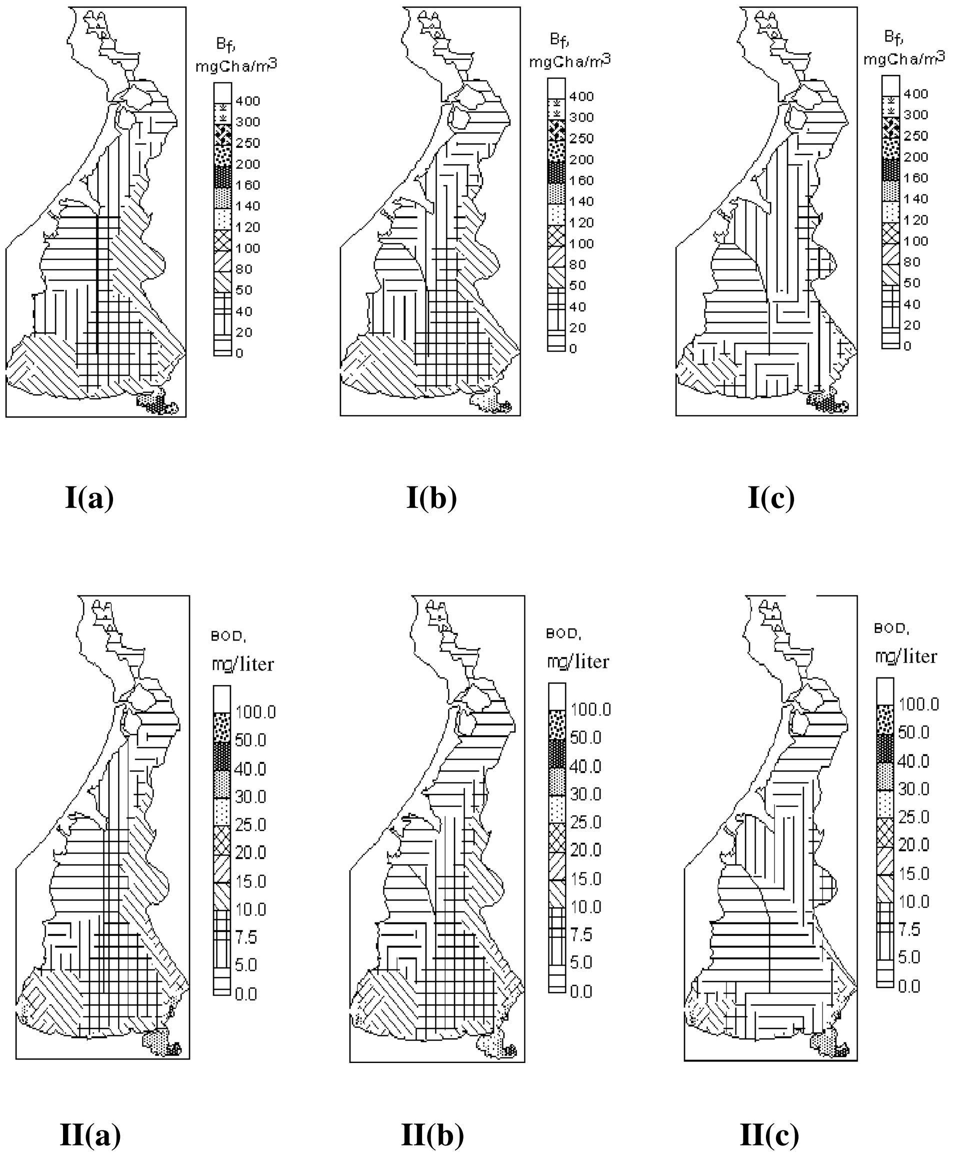


Fig. 7.22. Space distribution of the biomass of phytoplankton (I), in mg ChlA/ m^3, and the concentration of inert organic matter (II), in mg O_2/liter, determined on the basis of the model *for conditions of the humid season of 2025 in the case of the removal of 80% of discharge* and the construction of waterworks: cases 1 (a), 2 (b), and 3 (c).

The mathematical model was also used for the investigation of the appropriateness of construction of the indicated waterworks as the second turn of nature-conservation measures aimed at the improvement of water quality in the Ciénaga de Tesca lagoon and the restoration of its ecosystem.

The prognostic fields of the concentrations of chlorophyll *a,* inert organic matter (in BOD units), and ammonia nitrogen obtained on the basis of the model for conditions of 2025 in the case of the removal of 80% of the discharge of sources and the realization of the waterworks projects considered above are presented in Figs. 7.21–7.23. The analysis of results shows that the maximum effect of self-purification of the basin due to its hydrodynamic washing can be attained in cases 2 and 3. Since case 2 is more economical, on the basis of results of numerical experiments the following mixed mode of operation of channels was recommended: uncontrolled mode (case 2) in the dry period of a year, when strong trade winds dominate and the strait of natural origin in the north part of the basin is closed, and controlled mode (case 3) in the humid period of a year, when winds are weak and the north strait is open. In this case, the concentration of chlorophyll *a* in 2025 will decrease, on the average, to $30\ \mathrm{mg\ ChlA/m^3}$, the concentration of inert organic matter (BOD) will decrease to $7\ \mathrm{mg O_2}$/liter, and the concentration of ammonia nitrogen will decrease to a level below 0.1 mg N/liter.

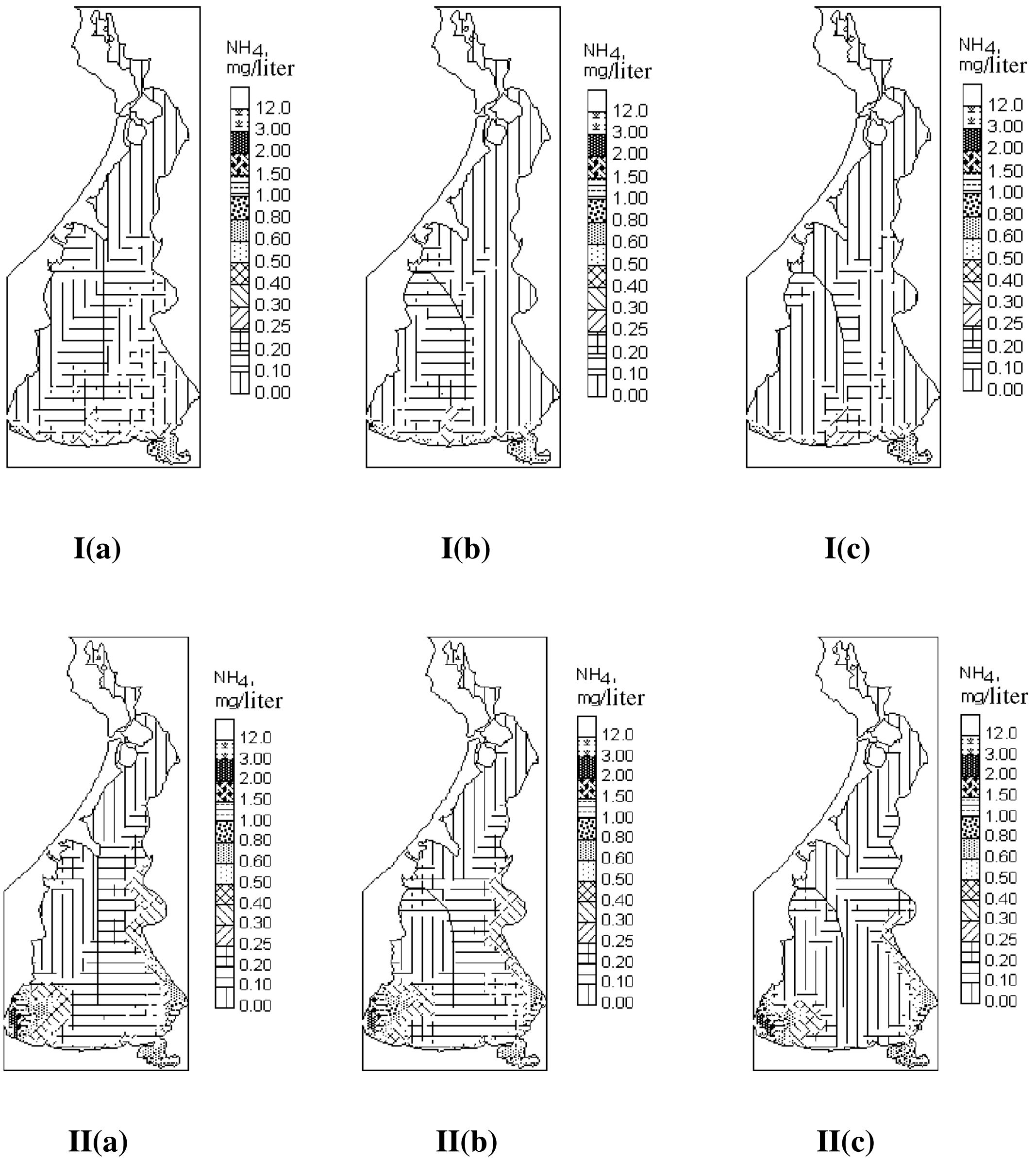


Fig. 7.23. Space distribution of ammonia nitrogen, in mgN/liter, determined on the basis of the model *for conditions of dry (I) and humid (II) seasons of 2025 in the case of the removal of 80% of discharge* and the construction of waterworks: cases 1 (a), 2 (b), and 3 (c).

7.5. Substantiation of the Strategy of Control of Water Quality in the Ciénaga Grande de Santa Marta Firth

The experience of engineering measures aimed at the reconstruction of the water exchange of Ciénaga Grande de Santa Marta with the sea and the Magdalena river through the Pajarales system of channels and lakes showed that the use of salinity as a unique criterion for the water quality of the firth is essentially wrong. The control of water quality in this ecosystem can give a positive result only if one takes into account the complex of all relationships between its biotic and abiotic components. In other words, the ecosystem approach to planning nature-conservation measures in the firth and in the Pajarales system of lakes should be realized. For this purpose, a two-dimensional mathematical model of the investigated ecosystem was developed. This model was used for the substantiation of the concept of control of water quality in the firth [97, 126].

This model was used for the solution of two main problems. The first problem was to evaluate the role of small rivers and water exchange with the Magdalena river through the Pajarales system of lakes in the formation of water quality of the firth. As potential pollution sources, the Fundación, Sevilla, Aracataca, and Aji rivers and the Grande, Tambor, and Clarin channels that connect the firth with lakes of the Pajarales system and, through them, with the Magdalena river, were considered. The concentration of pollutants in waters of all sources was taken equal to 100 c.u., which enables one to show the role of different sources in the pollution of the firth. At the initial time, the content of pollutants in waters of the firth was set equal to 10^{-12} c.u.

The level checkmarks at the external (open) boundaries of connecting channels and the flow rates of small rivers in different seasons of a year were taken from Tables 2.5–2.6.

The results of computations using the model of self-purification of waters from pollutants with different properties for conditions of July and October are presented in Figs. 7.24–7.25. The choice of these months is caused by the results of calibration of the two-dimensional version of the eutrophication model, according to which the situation observed in July corresponds to average annual conditions, and in October the discharge of small rivers and the inflow of waters of the Magdalena river through channels maximally affect the ecological situation in the firth.

We calculated the pollution of waters of the firth by toxic substances with the following properties:

(a) conservative dissolved substances whose concentration decreases only due to hydrodynamic dilution;

(b) nonconservative dissolved substances of “biologically rigid” type with the rate of destruction in the marine medium of order 10^{-7} sec^{-1} (e.g., fats and oils);

(c) nonconservative dissolved substances of “intermediate” type with the rate of destruction in the marine medium of order 10^{-6} sec^{-1} (e.g., phenols and detergents);

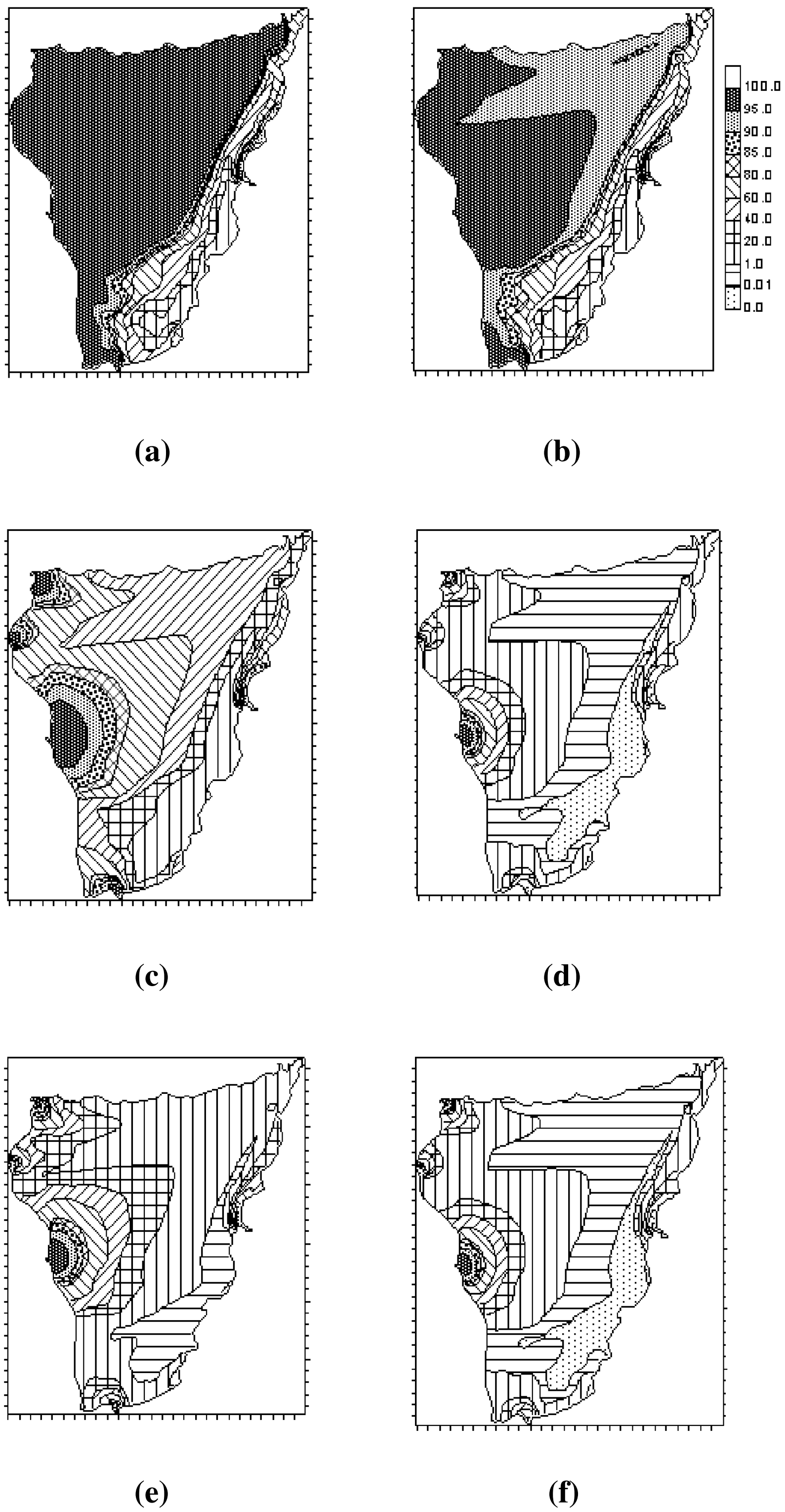


Fig. 7.24. Results of computation of the pollution of waters of the firth in a rainy season by conventional pollutants with the following characteristics: $w_{gi} = 0$, $K_{ci} = 0$ (a), $w_{gi} = 0$, $K_{ci} = 10^{-7}$ (b), $w_{gi} = 0$, $K_{ci} = 10^{-6}$ (c), $w_{gi} = 0$, $K_{ci} = 10^{-5}$ (d), $w_{gi} = 6.9 \cdot 10^{-6}$, $K_{ci} = 0$ (e), $w_{gi} = 6.9 \cdot 10^{-6}$ m/sec, $K_{ci} = 10^{-6}$ sec^{-1} (f).

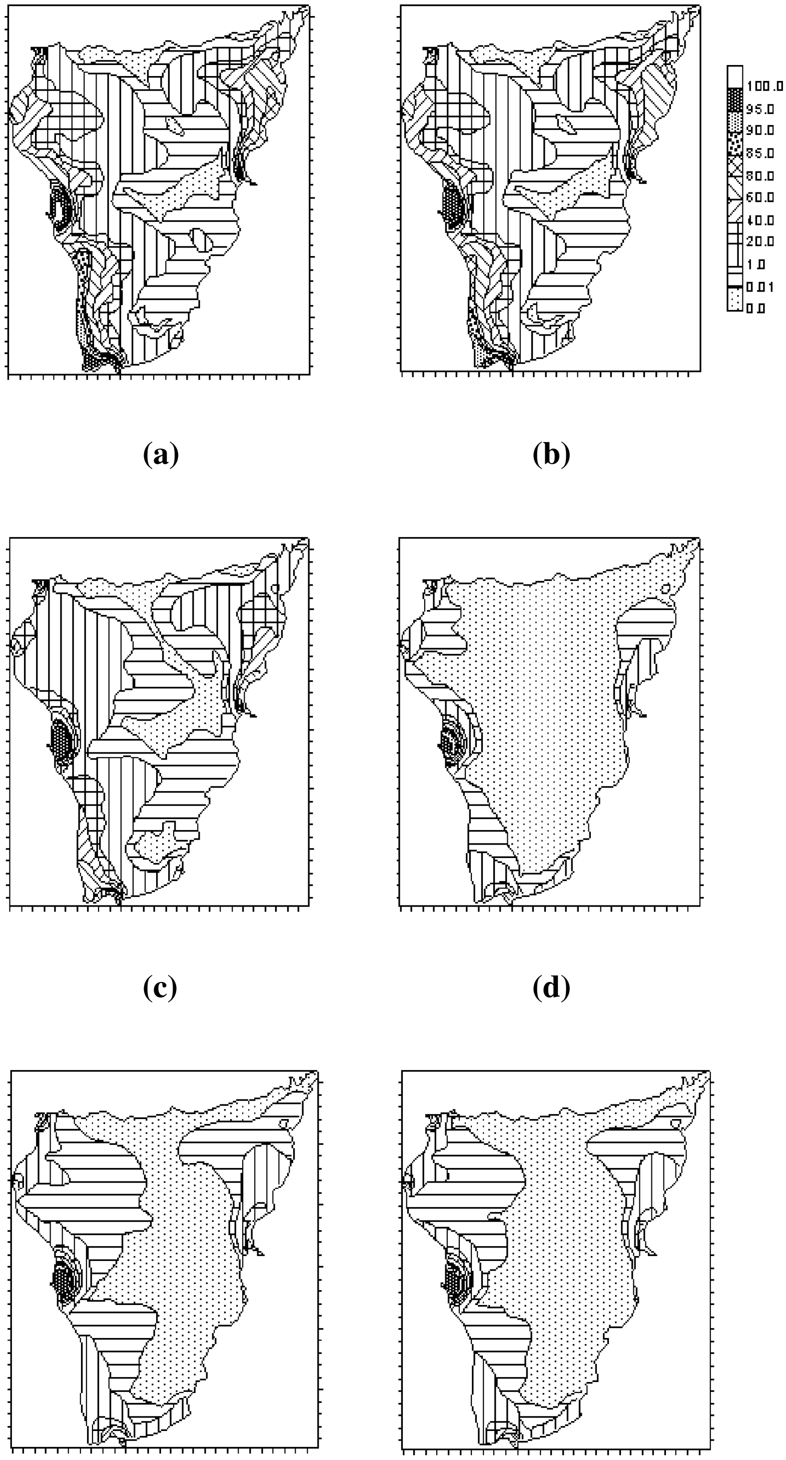


Fig. 7.25. Results of computation of the pollution of waters of the firth in July (transient season) by conventional pollutants with the following characteristics: $w_{gi} = 0$, $K_{ci} = 0$ (a), $w_{gi} = 0$, $K_{ci} = 10^{-7}$ (b), $w_{gi} = 0$, $K_{ci} = 10^{-6}$ (c), $w_{gi} = 0$, $K_{ci} = 0$ (d), $w_{gi} = 6.9 \cdot 10^{-6}$, $K_{ci} = 0$ (e), $w_{gi} = 6.9 \cdot 10^{-6}$ m/sec, $K_{ci} = 10^{-6}$ 1/sec (f).

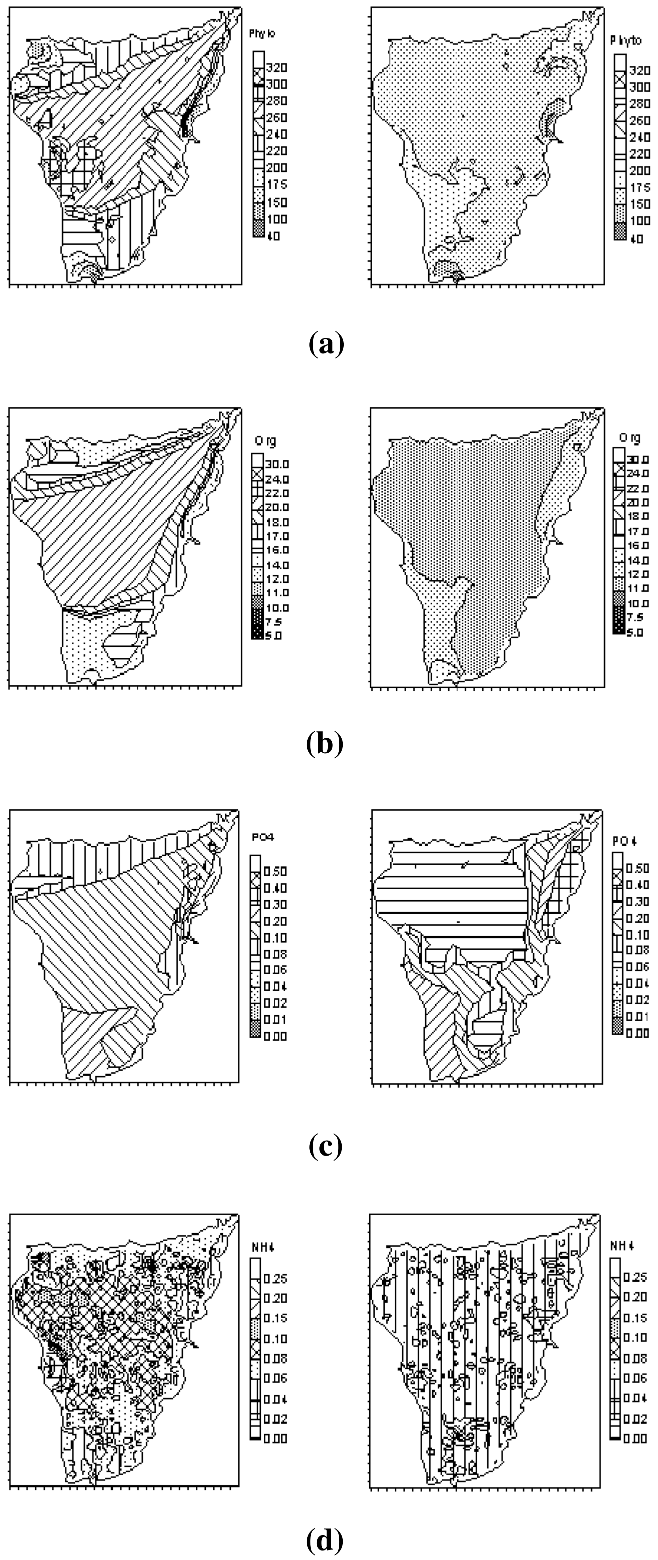


Fig. 7.26. Typical space distributions of the biomass of phytoplankton (a), in mg ChlA/m^3, the content of inert organic matter (b), in mg O_2/liter, phosphates (c), in mg P/liter, and ammonia nitrogen (d), in mg N/liter, in October (rainy season) corresponding to the present-data conditions (on the left) and to the case of the closure of the Grande, Tambor, and Clarin channels (on the right) computed on the basis of the model.

(d) nonconservative dissolved substances of "biologically soft" type with the rate of destruction in the marine medium of order 10^{-5} sec^{-1} and higher (e.g., pathogenic bacteria);

(e) conservative substances adsorbed to a suspension with the velocity of gravitational settling of particles of suspension of $6.9 \cdot 10^{-6}$ m/sec;

(f) nonconservative substances of "intermediate" type adsorbed to a suspension with the rate of destruction of order 10^{-6} sec^{-1} and the velocity of gravitational settling of particles of suspension of $6.9 \cdot 10^{-6}$ m/sec.

The obtained results (Figs. 7.24–7.25) show that the influence of the water exchange of the firth with the Magdalena river through the Pajarales system of small lakes on the operation of the ecosystem and its water quality is considerably greater than that of the discharge of small rivers. Therefore, to avoid excessive desalination and the rise of ground water in the banks of the firth in the rainy period, it is necessary to restrict the inflow of fresh water from the Magdalena river through the system of channels connecting the firth with small lakes. For the solution of this problem, it was proposed to construct controlled locks in the channels for maintaining the sea status of the water ecosystem in the firth and the fresh-water status in small lakes. This would enable one to preserve the fishery value of the lakes and fish farms raising oysters and shrimps in the water area of the firth. This would also lead to the creation of favorable conditions at the coast of the firth for the restoration of perennial mangrove thickets that grew there in earlier times.

The second problem solved with the use of the model is the prediction of the trophity level of waters of the firth in the case of closed locks in channels in the rainy season. The results of the computation, based on the eutrophication model, of parameters of the trophity level of waters of the ecosystem of the firth under the assumption that the Grande, Tambor, and Clarin channels are closed in the humid season of a year are presented in Fig. 7.23. One can see that, under this scenario of reconstruction of water balance of the firth, the ecological situation in it considerably improves due to a decrease in the content of mineral compounds of biogenic elements (e.g., the content of ammonia nitrogen decreases from 0.1 to 0.05 mgN/liter) in waters of the firth, which leads to a decrease in the biomass of phytoplankton (from 260 to 160 mg $ChlA/m^3$) and in the concentration of inert organic matter (from 21 to 11 mgO_2/liter). Therefore, the restriction of the amount of water of the Magdalena river that gets into the firth leads to a decrease in the eutrophication of the waters of the firth.

7.6. Evaluation of Appropriateness and Efficiency of Engineering Projects Aimed at a Decrease in the Inflow of Suspension and the Improvement of the Oxygen Conditions of Waters of the Cartagena Bay

As mentioned in Sec. 2.1.1, the household sewage of the town of Cartagena, the industrial sewage of enterprises of the industrial area of the town, and the navigation Dique

Channel more than 100 km long that connects the bay with the Magdalena river are the main sources of eutrophication and pollution of waters of the Cartagena Bay. For the prediction of ecological consequences and the evaluation of the efficiency of proposed engineering solutions of a wide range of economic and nature-conservation problems [143, 161, 164, 166], a three-dimensional mathematical water-quality model with eutrophication block of the third level of hierarchy was used.

The intensive inflow of suspended alluvia coming with the discharge of the Dique Channel is a serious problem for the operation of the Cartagena port complex. To decrease the amount of alluvia both in the channel itself and in the water area of the bay together with ship channels, engineering companies propose different projects of waterworks for the removal of a part of solid discharge of the channel with preservation of its flow rate and navigability. In this connection, there arises the problem of the prediction of ecological consequences of the realization of these waterworks projects for the ecosystem of the bay. Its solution was obtained with the use of the model of eutrophication and oxygen conditions of waters [96, 98, 166].

The aim of model experiments was to predict possible changes in the bioproductivity of the ecosystem and the oxygen conditions of waters of the bay caused by an increase in their transparency for different levels of purification of waters of the Dique Channel from the mineral suspension.

The concentration of mineral suspension in waters of the bay and its contribution to the decrease in the water transparency [see relation (5.5)] were preliminarily calculated in the self-purification block of the model. The transport of suspended alluvia was computed for three dimensional fractions of particles of alluvia whose characteristics are presented in Table 7.1. It was assumed that, in the total discharge of suspended alluvia of the Dique Channel, all dimensional fractions of particles are presented in equal proportions. The sand fractions of alluvia were not taken into account in computations because, due to high velocities of gravitational settling, they do not affect the field of water transparency in the bay except for a narrow local region near the mouth of the channel.

The influence of the present biomass of phytoplankton on the water transparency [see relation (5.6)] was taken into account in computations directly in the eutrophication block. Numerical experiments with model were carried out for extremal conditions of the rainy season, when the flow rate of the Dique Channel and the amount of suspension carried away with its waters are maximum, and oxygen deficiency occurs in the near-bottom layer. The following three situations were modeled:

(1) present-day situation corresponding to the humid season of a year (Fig. 2.4b);

(2) prognostic situation in the case where 50% of suspended alluvia that determine the water transparency in the bay are removed from waters of the Dique Channel;

(3) prognostic situation in the case of the removal of 90% of suspended alluvia that determine the water transparency in the bay.

Computed for these situations, the fields of water transparency determined only by the content of mineral suspension in waters of the bay are shown in Fig. 7.27. One can see that, in the case of removal of 50% of suspended alluvia, the field of water transparency approaches the field observed in a dry season (Fig. 2.4a), though the flow rate of the channel and, hence, the discharge of biogenic substances preserve values typical of the humid season. The removal of 90% of mineral suspension from waters of the channel leads to more radical changes. The water transparency of the bay does not decrease below 0.4 m even near the mouth of the Dique Channel, and, in some parts of the bay, it approaches the background values typical of the open sea.

Table 7.2. Characteristics of Suspended Alluvia (Silt) Coming with Discharge of the Dique Channel and Determining the Water Transparency in the Cartagena Bay

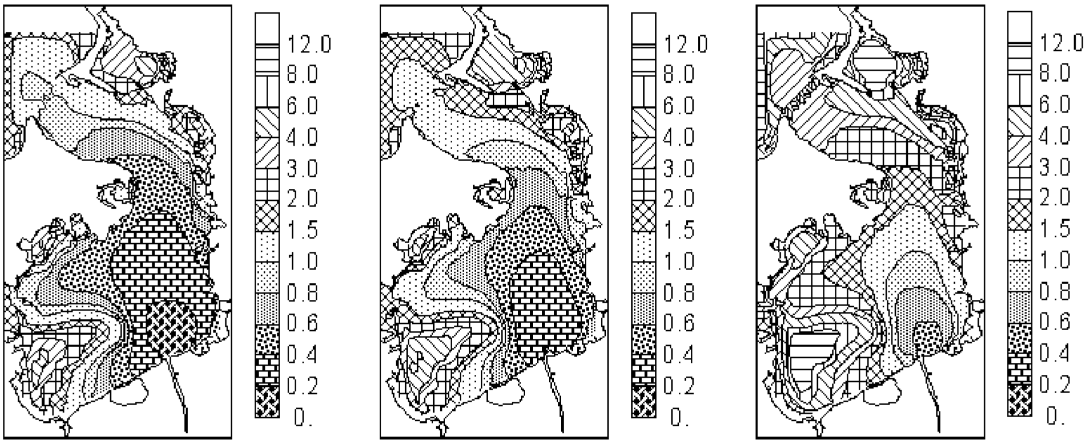
Characteristic of particles of silt, mm	Fraction, mm	Gravitational velocity, w_g m/sec	Concentration in waters of the channel, mg/liter
Large, 0.063	0.066–0.031	$3 \cdot 10^{-3}$	130
Medium, 0.005	0.031–0.016	$6 \cdot 10^{-4}$	130
Fine	0.016–0.008	$4 \cdot 10^{-5}$	130

For the correction of the flow of absorption of dissolved oxygen by bottom sediments in accordance with changes in the flow of organic matter into bottom sediments under new conditions, prognostic computations using the eutrophication model were performed in two steps. The aim of the first step was to determine a steady space distribution of chemical and biological variables of the state of the ecosystem of the bay under new conditions with preservation of previous (present-day) values of the flow of absorption of oxygen by bottom sediments. On the basis of the results of computation, the value of the flow of organic matter to bottom sediments in the predicted situation $F_{\text{org}}^{\text{new}}(x, y)$ was determined at every point of the computational region, and, on the basis of this value, the functional $f(x, y)$ in relation (4.46) was redefined as follows:

$$f(x, y) = \frac{F_{\text{org}}^{\text{new}}(x, y)}{F_{\text{med}}^{\text{act}}}.$$

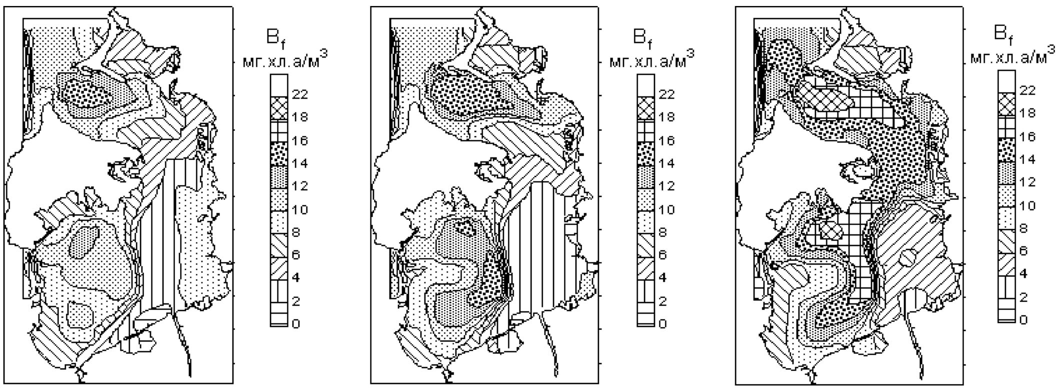
Then the prognostic computation was repeated with regard for the corrected flow of absorption of oxygen by bottom sediments $Q_{O_2}^{\text{bot}}$.

The results of computation performed on the basis of the eutrophication model for the considered situations are presented in Figs. 7.28–7.30. As expected, an increase in the water transparency of the bay with preservation of the values of concentrations of biogenic substances in waters of the channel leads to the growth of production and the biomass of phytoplankton in the photic layer of the bay. This results in an increase in the flow of organic matter to bottom sediments and the consumption of oxygen for its biochemical oxidation both in bottom sediments and in the near-bottom layer of waters of the bay. The areas of oxygen deficiency in the near-bottom layer formed under the present-day conditions in the humid season of a year become substantially wider and deeper in the modeling of prognostic situations.



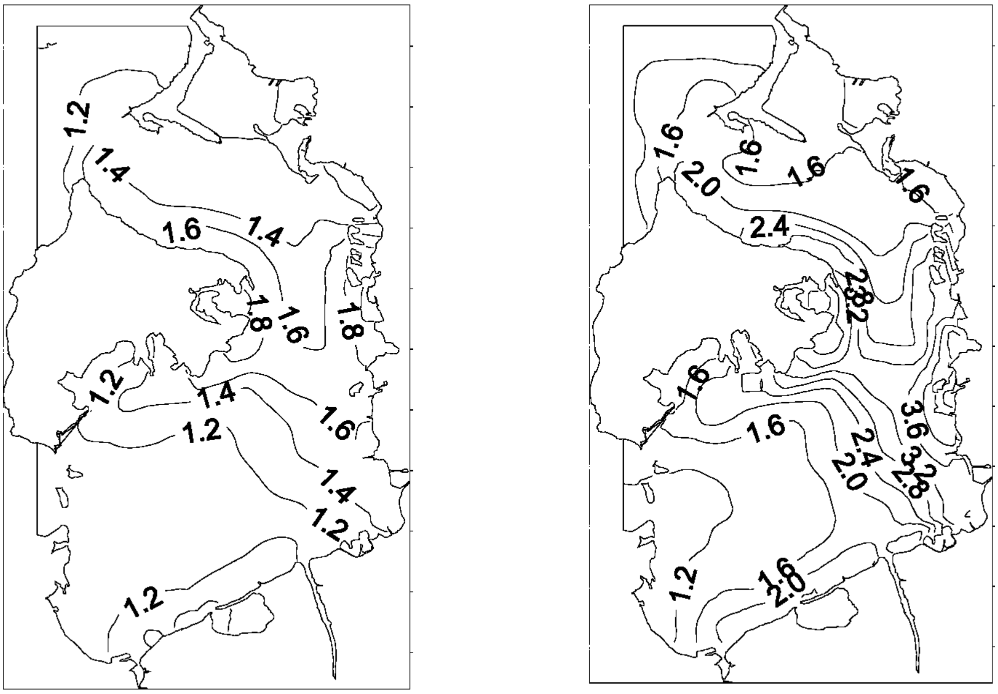
(a) **(b)** **(c)**

Fig. 7.27. Fields of water transparency (in meters) in the Cartagena Bay determined by the removal of suspension from the Dique Channel computed on the basis of the model for the present-day situation in the humid season (a) and in the cases of removal of 50% (b) and 90% (c) of the suspension.



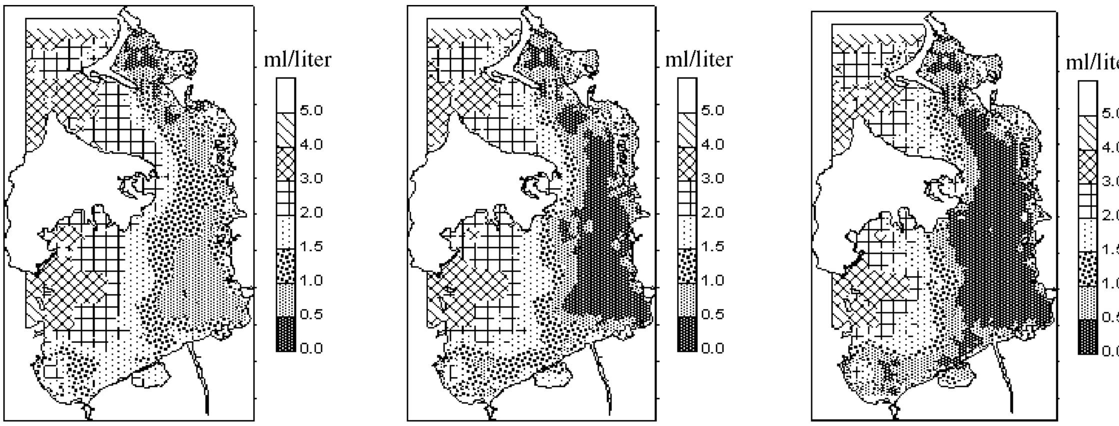
(a) **(b)** **(c)**

Fig. 7.28. Distribution of the biomass of phytoplankton, in mg ChlA/m^3, in the surface layer of the bay computed on the basis of the model for conditions of the humid season of a year for the present-day situation (a) and in the cases of removal of 50% (b) and 90% (c) of suspended alluvia from waters of the Dique Channel.



(a) **(b)**

Fig. 7.29. Distribution of the coefficients $k = F_{\text{org}}^{\text{new}} / F_{\text{org}}^{\text{act}}$ characterizing an increase in the flow of organic matter to bottom sediments in prognostic situations as compared with the present-day situation in the cases of removal of 50% (a) and 90% (b) of suspended alluvia from waters of the Dique Channel.



(a) **(b)** **(c)**

Fig. 7.30. Distribution of the content of dissolved oxygen, in ml/liter, in waters of the near-bottom layer of the Cartagena Bay in the humid season computed on the basis of the model for the present-day conditions (a) and in the cases of removal of 50% (b) and 90% (c) of suspended alluvia from waters of the Dique Channel.

In Sec. 2.1.1, we have noted that the appearance of hypoxic areas in the near-bottom layer of the Cartagena Bay in the humid season of a year is caused by the weak vertical mass and gas exchange determined by weak winds and the formation of a sharp near-surface pycnocline under the influence of the fresh discharge of the Dique Channel. Biogenic substances that come with river waters spread within the limits of the surface desalinated layer of the bay (which is simultaneously photic). The content of biogenic substances in waters of the channel is considerably higher than in near-shore sea waters. Thus, the channel is a powerful source of biogenic substances and favors the eutrophication of waters of the bay.

On the other hand, the mineral suspension that gets into the bay with waters of the channel considerably decreases the seawater transparency and, hence, restrains the process of primary production of organic matter by phytoplankton, simultaneously strengthening the role of the hydrodynamic process of dilution of polluted river waters by relatively clear sea waters. If a part of the mineral suspension coming from the channel is removed, then the existent balance between the contributions of the discharge of the Dique Channel to the stimulation of photosynthesis and to its restriction is violated toward the first one, and, as a result, the oxygen conditions of the bay deteriorate.

On the basis of the results obtained, it was concluded that a partial removal of suspended alluvia from waters of the Dique Channel leads to the deterioration of the ecological situation and water quality in the Cartagena Bay caused by an increase in the primary production and concentration of organic matter in water and bottom sediments and the intensification of hypoxic phenomena in the near-bottom layer. This conclusion forced experts to seek other, more complex, methods for the solution of the problem of decrease in the solid discharge of the Dique Channel, combining them with the necessity of decreasing the biogenic discharge of the channel and the improvement of the oxygen conditions of waters of the bay.

With regard for the arguments presented above, the following ideas of the solution of the problem seem to be the most promising:

(i) decrease the flow rate of the Dique Channel in the humid season of a year in the region of its inflow to the Cartagena Bay by building a lock that redistributes the discharge of the channel to its other armlets falling into the open sea [161];

(ii) decrease the content of biogenic substances in waters of the channel, preliminarily passing them through the system of natural lakes accompanying the Dique Channel along its entire length and connected with one another by a system of canals;

(iii) in view of the fact that the Dique Channel has lost its former importance as a transport communication for the Cartagena Port, completely close its outlet to the bay and redistribute the discharge to other armlets falling into the sea.

The efficiency of these scenarios was evaluated by using the mathematical model of eutrophication on the basis of the degree of their influence on the improvement of the oxygen conditions of the Cartagena Bay, the most vulnerable element of the ecosystem, and the integral index of its water quality.

The modeling of the last, most radical, scenario assuming the complete closure of the Dique Channel with preservation of the present-day discharge of waters polluted by anthropogenic sources showed that the expected improvement of the situation would not occur (Fig. 7.33b). This is explained by the fact that, as a result of the closure of the channel, the water transparency of the bay increases to 6 m and ceases being a factor that restricts photosynthesis, whereas the inflow of mineral compounds of biogenic elements and organic matter from anthropogenic sources (see Sec. 2.1.1) located at the shores of the bay continues the stimulation of the development of phytoplankton and the appearance of hypoxia areas in the near-bottom layer. These results allow one to conclude that the restriction of discharge of biogenic substances by anthropogenic sources is the main condition for the solution of the problem of improvement of oxygen conditions of waters of the bay.

According to the plan of development of the town of Cartagena, it is assumed that, by 2025, all household sewer systems of the town will be combined into a central sewer system with discharge into the open sea far from the town. It is planned to reduce the discharge of mineral compounds of biogenic elements and inert organic matter by enterprises of the industrial area by 80%. The modeling of this scenario showed that the indicated measures enable one to avoid the formation of oxygen deficiency in the near-bottom layer of the Internal Bay (Figs. 7.31c, 7.32b, and 7.33c). In the External Bay, despite a certain decrease in the oxygen deficiency, the situation does not change qualitatively because, as before, the content of oxygen in the near-bottom layer of the most part of the water area remains below 1.5 ml/liter. This is explained by the fact that, despite a considerable decrease in the discharge of anthropogenic sources, the main cause of the formation of oxygen deficiency (the removal of fresh waters with high content of biogenic substances from the Dique Channel, the formation of a strong near-surface pycnocline, and, as a result, a weak ventilation of the near-bottom layer of the bay with oxygen) is not eliminated. For this reason, in addition to the ideas presented above, three integrated complex scenarios (alternatives) were considered. In all these scenarios, the first step of nature-conservation measures is the complete removal of household sewage and the 80% removal of the industrial discharge of the town of Cartagena, and only at the second step one passes to the realization of the following engineering solutions, considered above and aimed at the restriction of discharge and improvement of water quality of the Dique Channel:

(1) a decrease in the flow rate of the Dique Channel in the humid period of a year from 150 to 50 m^3/sec (the flow rate during a dry season);

(2) a decrease in the flow rate of the Dique Channel in the humid period of a year from 150 to 50 m^3/sec and a twofold decrease in the content of mineral compounds of nitrogen and phosphorus in waters of the channel;

(3) the complete closure of the channel.

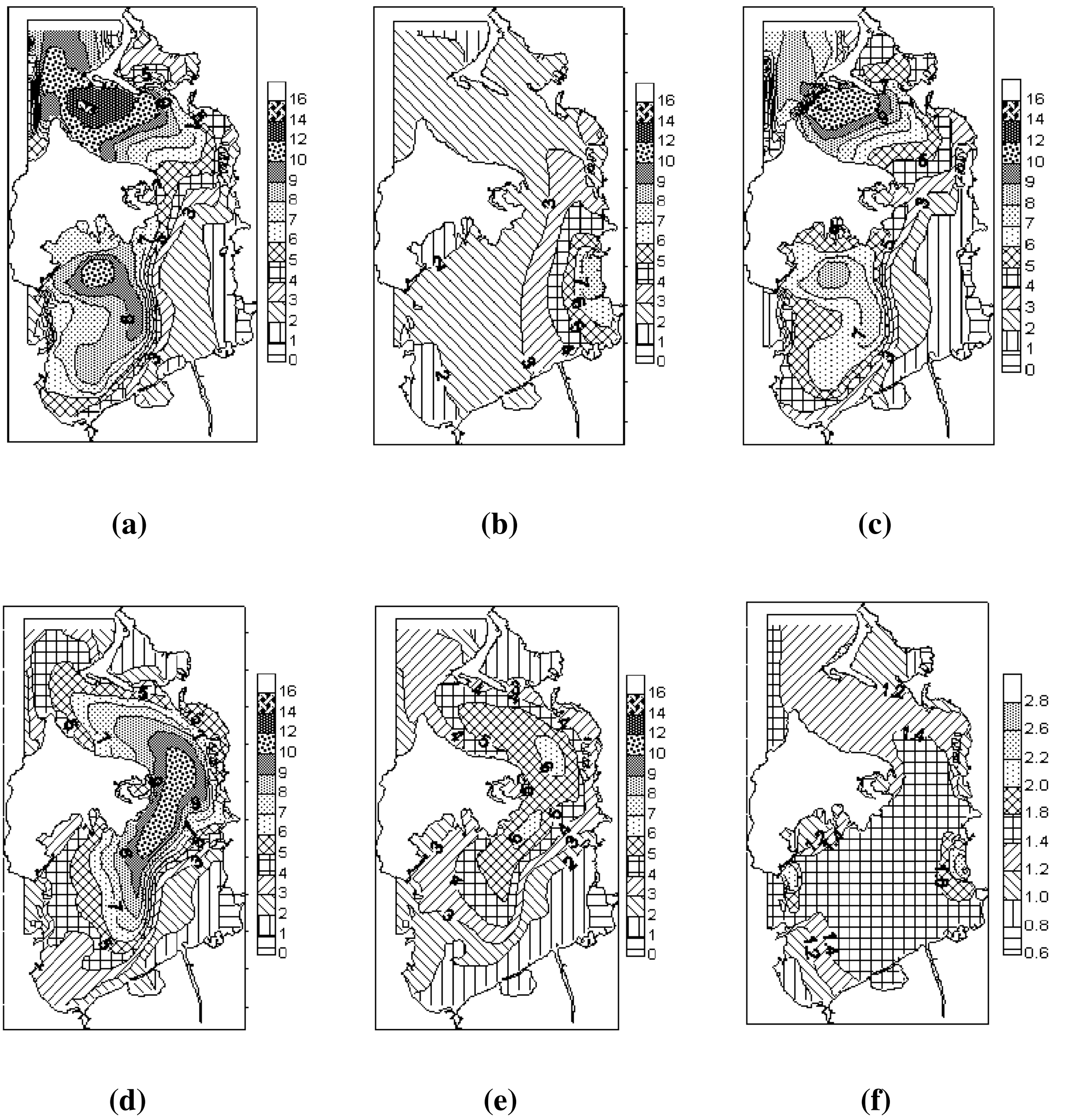


Fig. 7.31. Distribution of the biomass of phytoplankton, in mg ChlA/m^3, in the surface layer of the Cartagena Bay in the humid season of a year obtained on the basis of the model for the present-day conditions (a), the closure of the Dique Channel (b), the removal of 100% of household and 80% of industrial discharge of the town (c), the removal of discharge (case (c)) and the restriction of the flow rate of the channel to 50 m^3/sec (d), the previous case with additional twofold decrease in the content of biogenic substances in waters of the channel (e), and the removal of discharge (case (c)) and the closure of the channel (f).

As the flow rate of the channel decreases to 50 m^3/sec, the amount of suspension removed from the channel decreases and the water transparency of the bay increases. This effect is taken into account by specifying the field of transparency typical of a dry season. As the water transparency increases, the primary production of phytoplankton increases and the flow of organic matter to bottom sediments from the central part of the bay, where the oxygen content is minimum, becomes more intensive (Figs. 7.31d, 7.32c, and 7.33d).

Thus, a partial removal of the discharge of the channel, similarly to the case of the removal of a part of suspended alluvia considered above, does not advance the improvement of the oxygen conditions of the bay because, as before, the channel remains a strong source of biogenic substances, and the areas of maximum production of phytoplankton move from the boundaries of the water area to the central part of the bay.

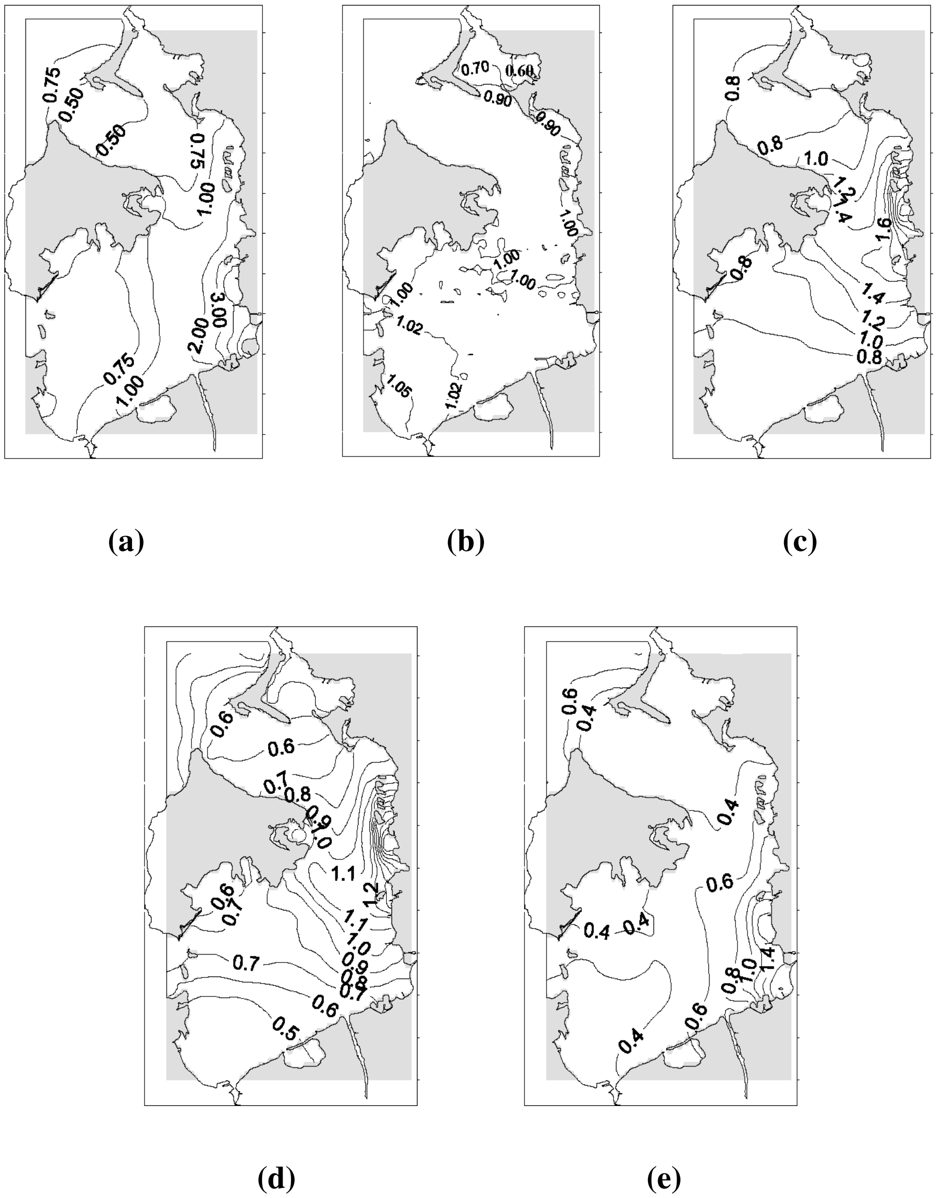


Fig. 7.32. Distribution of the coefficients $k = F_{\text{org}}^{\text{new}} / F_{\text{org}}^{\text{act}}$ characterizing variations in the flow of organic matter to bottom sediments in prognostic situations as compared with the present-day situation in the case of the closure of the Dique Channel (a), the removal of 100% of household and 80% of industrial discharge of the town (b), the removal of discharge and restriction of the flow rate of the channel to 50 m^3/sec (c), the previous case with additional twofold decrease in the content of biogenic substances in waters of the channel (d), and the removal of discharge and the closure of the channel (e).

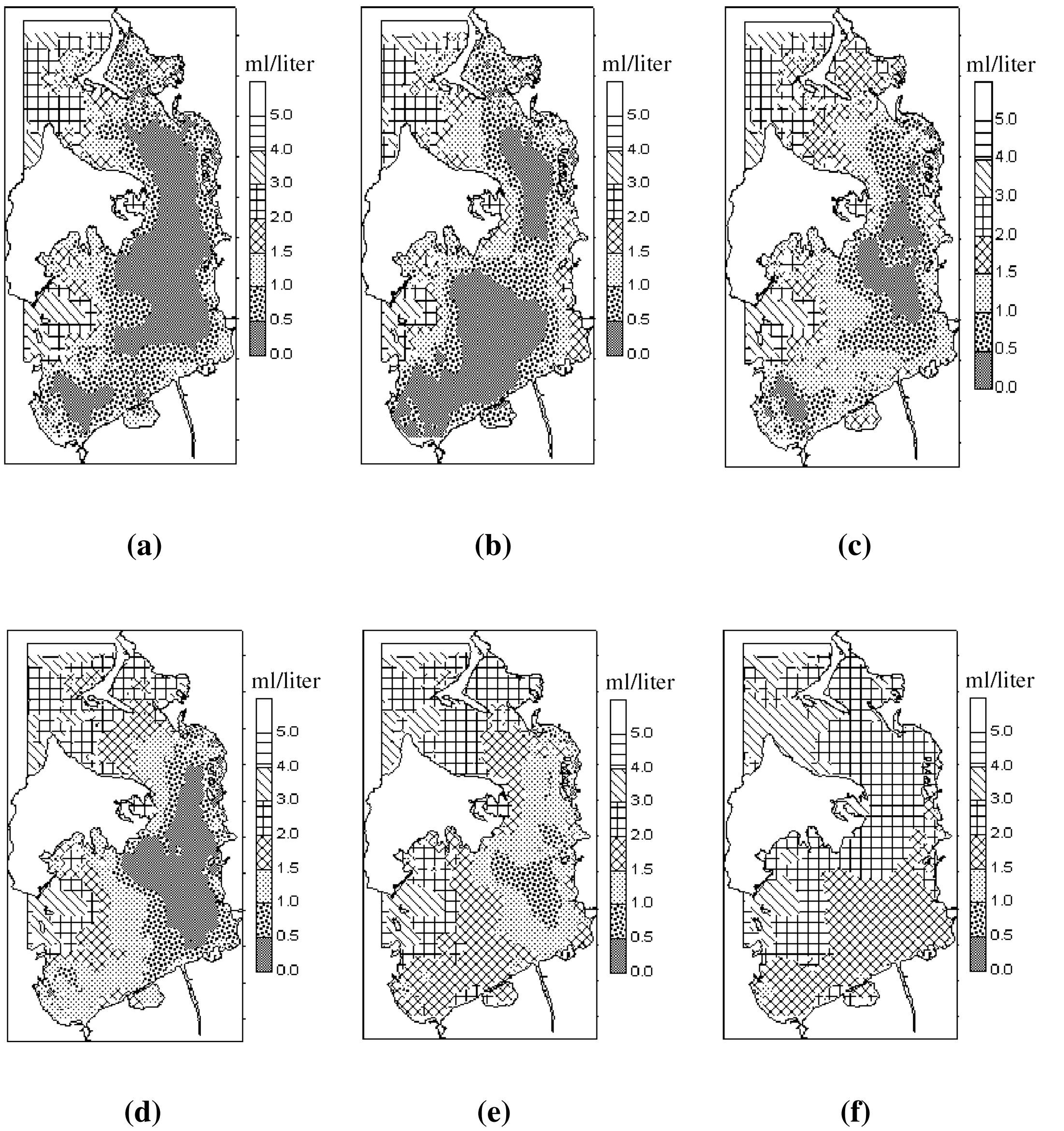


Fig. 7.33. Distribution of oxygen, in ml/liter, in the near-surface layer of the Cartagena Bay in the humid season of a year determined on the basis of the model for the present-day conditions (a), the closure of the Dique Channel (b), the removal of 100% of household and 80% of industrial discharge of the town (c), the removal of discharge (case (c)) and the restriction of the flow rate of the channel to 50 m^3/sec (d), the previous case with additional twofold decrease in the content of biogenic substances in waters of the channel (e), and the removal of discharge (case (c)) and the closure of the channel (f).

A decrease in the content of biogenic substances in waters of the channel, together with the restriction of its discharge to 50 m^3/sec, gives much better results. In the most part of the water area of the bay, the biomass of phytoplankton and bacterioplankton, as well as the flow of organic matter to bottom sediments, substantially decrease, and, as a result, the oxygen deficiency in the near-bottom layer decreases (Figs. 7.31e, 7.32d, and 7.33e).

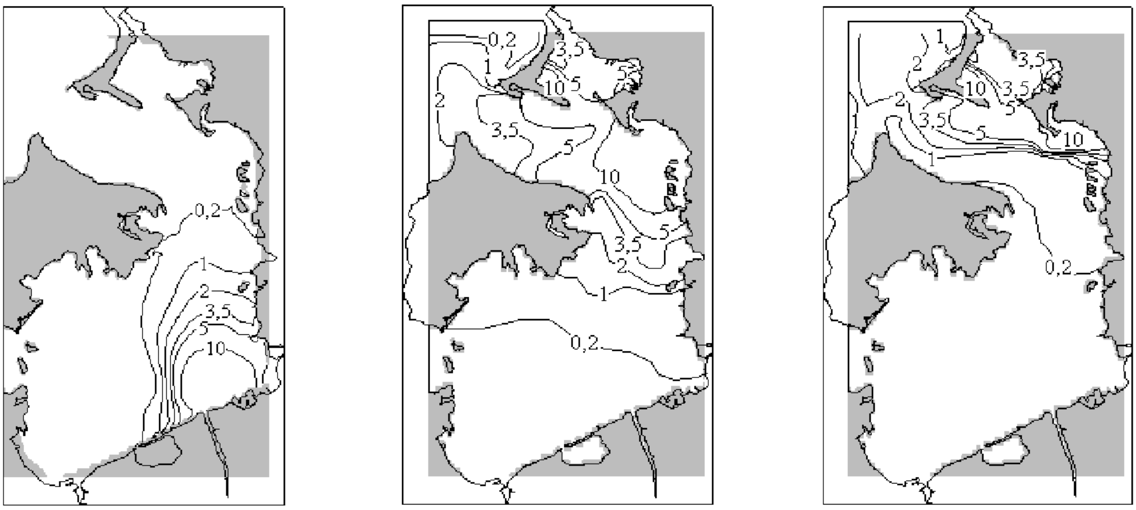
In the case of the complete closure of the channel, the trophic status of waters of the bay maximally approaches the status of seawater, and the oxygen deficiency in the near-bottom layer disappears (Figs. 7.31f, 7.32e, and 7.33f). In the southern part of the External Bay, which is weakly washed by oceanic waters and in which a group of industrial sources with large discharge of polluted waters is located (even under the conditions of removal of 80% of their present-day discharge), the content of oxygen in the near-bottom layer in the humid season of a year increases to 1.5 ml/liter, whereas in the Internal Bay it increases to 2.5 ml/liter.

Thus, the simulation of different scenarios of the improvement of oxygen conditions in the Cartagena Bay by using the mathematical model of eutrophication of waters shows that the general strategy should be aimed at the successive regulation of and decrease in the discharges of municipal household and industrial sources of pollution of waters of the bay accompanied by the maximum possible restriction of discharge of the Dique Channel and a decrease in the content of biogenic substances in its waters.

The second circle of problems solved with the use of the water-quality model dealt with the evaluation of the scale and level of pollution of waters of the Cartagena Bay on the basis of information on the content of pollutants in waste waters. The aim of these computations was to reveal the role of separate anthropogenic sources in the formation of the total level of pollution of waters of the bay and to develop requirements and recommendations for the organization and realization of ecological monitoring and the regulation of discharge of pollutants into waters of the bay.

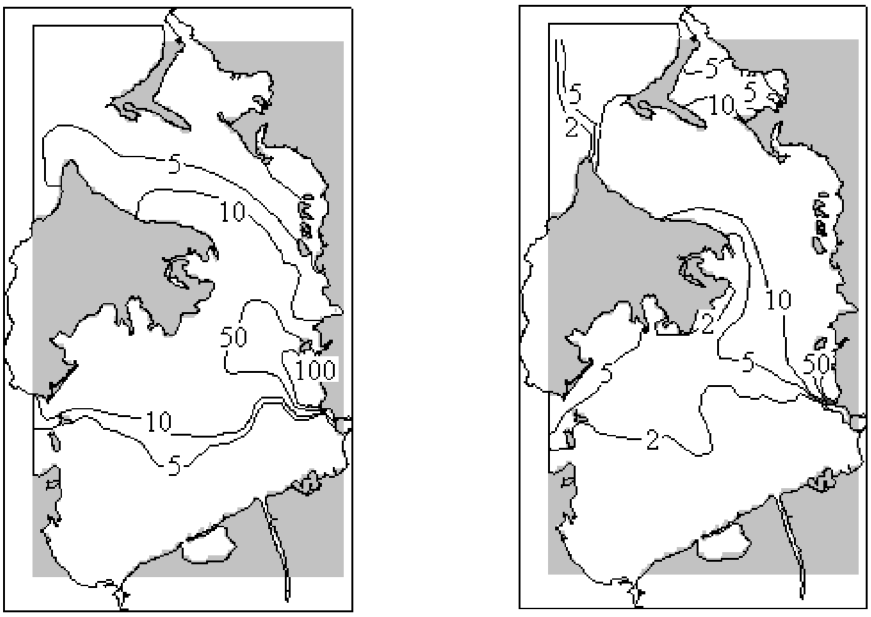
With regard for the recreation value of the northern part of the External Bay and especially of the water area of the Internal Bay of Cartagena, of special importance is the problem of the water-quality control of the bay aimed at the prevention of its pollution with pathogenic bacteria. The sources of the inflow of pathogenic bacteria to waters of the bay are the raw household sewage of the town (Fig. 2.3 and Table B.2) and the Dique Channel, into which many adjacent farms and villages discharge raw waste waters. The average amount of fecal coli-forms in household sewage is 10^8 microorganism/100 ml, whereas the maximum value observed in the waters of the Dique Channel is equal to 10^6 microorganism/100 ml.

Computations based on the water-quality model with self-purification block [see relation (4.4)] showed that the household sewage of the town is the main pollution source in the north part of the bay (Fig. 7.34). Thus, the level of pollution of the water area of the Internal Bay can exceed the allowable limits (200 microorganism/100 ml) all over the year. The Dique Channel does not play a significant role in the pollution of the central and northern parts of the bay, which is explained by the high mortality of colon bacillus in the surface layer of the bay under the existing conditions of marine medium (high water temperature, influence of sunlight, and mixture with salt seawater). In the dry period of a year, the pollution of waters of the bay with colon bacillus is higher than in the humid season (Fig. 7.34). This is explained by the fact that, in the dry season, under the influence of strong north tradewinds, the circulation of surface waters facilitates the accumulation of fecal coli-forms inside the bay. Conversely, in the humid season, waters polluted with colon bacillus are carried away from the bay through the northern strait.



(a) **(b)** **(c)**

Fig. 7.34. Pollution of surface waters of the Cartagena Bay by fecal coli-forms ($\times 10^3$ microorganism/100 ml) arriving with waters of the Cartagena Bay in the rainy season (a) and with waste waters in the dry (b) and humid (c) seasons computed on the basis of the self-purification model.



(a) **(b)**

Fig. 7.35. Pollution of waters of the bay with phenols, in µg/liter, in the dry (a) and humid (b) seasons of a year computed on the basis of the model for the coefficient of nonconservativeness K_{cf} = $1.9 \cdot 10^{-6}$ sec^{-1}. The concentration in the source is equal to 0.56 mg/liter.

The results of modeling made it possible to systematize and analyze data of episodic observations [165] of the level of pollution by pathogenic microflora in the water area of the Cartagena Bay. As a result, it was recommended to perform regular monitoring of water quality with respect to pathogenic microorganisms in the beach complexes of the series of hotels located at the Bocagrande spit, which separates the Internal Bay from the open sea and the External Bay (Fig. 2.3).

On the basis of results of model computations (Fig. 7.35) and information on the content of phenols in waste waters of one of the plants of the industrial area of the town of Cartagena, it was concluded that the content of these substances in seawater in the regions of location of beaches can exceed, especially in the rainy season, the national maximum allowable norms (2 μg/liter for areas of direct contact of humans with water), and it was recommended to include observations of the concentration of phenol to the system of ecological control of water quality of the bay.

The last examples illustrate the possibilities of application of mathematical models to the planning of ecological monitoring of near-shore marine water areas subject to the action of anthropogenic pollution sources.

Conclusions

Mathematical water-quality models can be efficiently used for the solution of a broad range of applied problems related to development of an optimal strategy of control of water quality of coastal marine water areas subject to anthropogenic load. They enable one to make an objective prediction of the development of ecological situation under variation in external loads acting on the ecosystem and to determine the scale and level of pollution of the investigated marine water areas both by individual local sources of the inflow of pollutants to the marine medium and by their combination.

Using specific examples, we have illustrated methodological approaches to the solution, with the use of numerical mathematical models, of the following applied problems of control of water quality of shelf marine ecosystems subject to a strong anthropogenic load:

(i) the determination of relative contributions of coastal anthropogenic sources and river discharge to the observed level of pollution of marine water areas aimed at the evaluation of the controllability of water quality of the shelf marine ecosystem (by example of the Odessa region of the northwest part of the Black Sea);

(ii) the choice of the region of location of a pollution source according to the criterion of minimization of the predicted level of pollution in nature-conservation marine are (by example of an oil terminal in the Odessa region of the northwest part of the Black Sea);

(iii) the development of a strategy of improvement of water quality of partially and periodically completely isolated marine water areas (basins) with regard for actual possibilities:

(a) regulation of discharges of pollutants by coastal anthropogenic sources (by example of the tropical Siénaga de Tesca lagoon and the Cartagena Bay);

(b) intensification of washing of the water area and water exchange with open sea by means of construction of various waterworks, e.g., connecting channels and directional jetties (by example of the tropical Siénaga de Tesca lagoon and the Tuzla firths of the northwest part of the Black Sea);

(iv) the evaluation of the efficiency of engineering measures aimed at the improvement of water quality and a decrease in the level of sediment accumulation in marine basins of estuary type by means of regulation of river, terrigenous, and biogenic discharge (by example of the Cartagena Bay and the Ciénaga Grande de Santa Marta Firth);

(v) the evaluation of the efficiency of various nature-conservation projects aimed at the improvement of oxygen conditions of near-bottom waters of deep, partially isolated marine water areas (by example of the tropical Cartagena Bay);

(vi) the application of results of mathematical modeling of propagation and transformation of pollutants in the marine medium to the assessment of the level and scale of pollution of the water area by individual local sources of pollution or by their group and to the planning of ecological monitoring (by example of the Cartagena Bay, the Ciénaga Grande de Santa Marta Firth, and the Dnieper–Bug and Odessa regions of the northwest part of the Black Sea).

For the investigated shelf marine water areas, on the basis of results of numerical experiments with modifications of the water-quality model, optimal strategies of realization of engineering and nature-conservation projects aimed at the improvement of quality of the water medium were determined. These strategies are as follows:

(i) for the Cartagena Bay: the maximum possible restriction of discharge of the Dique Channel and a decrease in the content of biogenic substances in its waters accompanied by the minimization of discharge of coastal anthropogenic sources of the town of Cartagena by means of construction of a centralized sewer system with outlet to the open sea;

(ii) for the Ciénaga de Tesca lagoon: the top-priority partial removal of household sewage of the town of Cartagena by means of construction of a centralized sewer system with subsequent construction of a system of waterworks consisting of two connecting channels and a directional jetty between them aimed at the intensification of hydrodynamic washing of the basin with relatively clear sea water;

(iii) for the Ciénaga Grande de Santa Marta Firth: the construction of a system of locks in channels that connect the firth with the system of small lakes and the Magdalena river aimed at the control of the inflow of river waters to the firth and the maintenance of the marine status of its ecosystem;

(iv) for the Odessa region of the northwest part of the Black Sea: the regulation of discharge of phosphorus-containing pollutants by coastal anthropogenic sources in the spring season of a year, the inadmissibility of discharge of waste waters from the "Severnaya" station of biological purification to the near-shore area of the sea in summer, and the improvement of the quality of river waters of the Dnieper and Yuzhnyi Bug for the radical change in the ecological situation in the region on the whole;

(v) for the Tuzla group of firths of the northwest part of the Black Sea: their transformation into an open marine basin with high degree of water renewal and water quality close to the marine one by means of construction of two channels at the opposite sides of the sand bay bar for connection with the sea.

CONCLUSIONS

In this work, we have presented results of experimental investigation and a theoretical generalization for a solution of the scientific problem of evaluation of actual possibilities of control over the water quality of ecosystems of shelf areas of seas of temperate and tropical latitudes subject to strong anthropogenic load on the basis of analysis of data of many-year ecological monitoring and results of numerical mathematical modeling. We have shown that mathematical water-quality models for marine ecosystems are an efficient tool for ecological planning, prediction, and evaluation of the suitability and propriety of various executive solutions in the field of the use and conservation of resources of the marine medium.

The main scientific and practical results of the work are the following:

1. On the basis of a system analysis of data of ecological monitoring for 1988–1999, we obtained new information on operating hydrochemical characteristics of the Odessa region of the northwest part of the Black Sea and showed their relationship with river discharge, hydrological conditions and phenomena, and modes of operation of anthropogenic pollution sources in the near-shore area. We established the following:

— in the spring–summer period of a year, the production of phytoplankton in the marine part of the water area can be limited by the concentration of mineral phosphorus;

— the concentrations of phosphates and ammonia in the near-shore area of the sea are, as a rule, considerably higher than in the marine part of the water area, which is explained by the influence of coastal anthropogenic sources and specific features of hydrological conditions;

— frequent, intensive, and long-term penetration of the tongue of desalinated waters from the Dnieper–Bug Firth in spring and the development of coastal wind upwelling in the spring–summer season of a year facilitate the intensification of the process of eutrophication of waters and the development of hypoxia in the near-shore area.

2. For the first time, on the basis of data of monitoring, we performed a systems analysis of the present-day ecological state of tropical basins of the Colombian Coast of the Caribbean Sea subjected to strong anthropogenic influence: the shallow Ciénaga de Tesca lagoon, the estuary-type Ciénaga Grande de Santa Marta lagoon, and the deep sea Cartagena Bay. We established the following:

— in the near-bottom layer of the Cartagena Bay, an extensive hypoxia occurs in the humid season of a year, which is caused equally by the discharge of raw household and industrial sewage of the town and by the inflow of polluted fresh waters of the Magdalena river through the Dique Channel, combined with specific features of the wind conditions and the morphology of the basin;

— as a result of the systematic discharge of raw household sewage of the town of Cartagena to the shallow Ciénaga de Tesca lagoon, the latter became a hypertrophic polysaprobic basin with violated natural balance of production–destruction processes and symptoms of instability in the dynamics of the ecosystem;

— the unrestricted inflow of fresh waters from the Magdalena river to the Ciénaga de Santa Marta Firth through a system of canals in the humid season of a year produces a negative effect on the quality of its waters and leads to the development of eutrophication and unfavorable conditions for raising valuable marine cultures and restoration of perennial mangrove thickets.

3. For the first time, we have developed the methodological support for the technological chain of applied ecological modeling of seawater quality: ecological monitoring—statement of the problem—development of an adequate mathematical model—its calibration and verification—numerical experiments—scientifically substantiated recommendations on the preservation and improvement of the quality of marine medium and its resources.

4. For the first time, we have developed a three-dimensional nonstationary applied water-quality model of shelf marine ecosystems, which can be used for the computation of the dynamics of waters and the formation of a thermohaline structure and water quality on water areas of water objects whose separate regions have a subgrid space scale along one of the horizontal coordinates (mouths of rivers, narrow straits, channels, etc.). This model is realized in a coordinate system curvilinear with respect to the vertical line and is equipped with eutrophication blocks of different levels of complexity of organization, the block of self-purification of waters from pollutants of various types, and the block of assimilation of hydrometeorological information at the boundaries of the computational domain. The possibility of making prompt changes in the complexity and working mathematical structure of the model according to the aims and conditions of computation is implemented.

5. We have developed a hierarchical complex of eutrophication blocks with original mathematical structure that differ in the number of variables and the level of specification

of correlations between biotic and abiotic components of a marine ecosystem (model). This complex enables one to describe, adequately and with minimum costs for ecological monitoring, the space–time variability of water-quality parameters in marine water areas with different degrees of eutrophication of waters. Recommendations for the use of each block are given. We have proposed a new scheme for the introduction of bacterioplankton into the structure of the eutrophication block and a concept of development of a water-quality model to the level of a complex model of operation of a water ecosystem and an ecotoxicological model.

6. We have developed requirements for the organization and structure of ecological monitoring of marine medium, including specialized experiments motivated by the necessity of information support of the process of development, adaptation, calibration, and application of water-quality models to the solution of practical problems of oceanology and sea ecology. We have determined, systematized, and developed methodological approaches to the determination of parameters of the water-quality model from results of ecological monitoring.

7. We have generalized and systematized results of various investigations for the determination of typical values of the rates of chemical and biological processes that are taken into account in models of water quality of marine and fresh-water ecosystems, ranges of their variability, and dependences on characteristics of the water medium.

8. We have developed original schemes and methods for the calibration of eutrophication blocks of the water-quality model, which successfully passed testing and showed their efficiency in the solution of applied problems for marine water areas and basins in various climatic zones having different morphological, hydrological, hydrochemical, and hydrobiological characteristics.

9. We have developed and improved a methodology of application of numerical mathematical models to the determination of an optimal strategy of control of water quality of shelf marine ecosystems subjected to strong anthropogenic influence by solving the following applied problems of oceanology and sea ecology:

— the determination of relative contributions of regulated and unregulated sources to the observed level of pollution of marine water areas aimed at the evaluation of the degree of controllability of the water quality of a marine ecosystem;

— the determination of the level and scale of pollution of the marine medium by local pollution sources and the role of some local sources in the formation of the quality of the marine system;

— the choice of the region of location of a pollution source according to the criterion of minimization of the predicted level of pollution in nature-conservation marine areas;

— the development of the strategy of improvement of the water quality of partially and (or) periodically isolated marine water areas (basins) with regard for actual possibilities: the regulation of discharge of pollutants by coastal anthropogenic sources and the intensification of washing of the water area and water exchange with the open part of the sea by means of construction of various waterworks;

— the assessment of the efficiency of engineering measures aimed at the following:

(i) the improvement of water quality and a decrease in the level of sediment accumulation in marine basins of estuary type by means of regulation of flow rates and terrigenous and biogenic discharge of river waters;

(ii) the improvement of oxygen conditions in near-bottom waters of partially isolated deep marine water areas.

10. For each shelf marine water area investigated in this work, on the basis of results of numerical modeling with modifications of the water-quality model, we have determined optimal strategies for the realization of nature-conservation measures aimed at the improvement of quality of the water medium:

— for the Cartagena Bay: the complete removal of household sewage and partial removal of industrial sewage of the town (by means of construction of a centralized sewer system) combined with maximum possible restriction of the inflow of fresh waters of the Magdalena river through the Dique Channel (by means of construction of a lock) and a decrease in the content of biogenic substances in these waters (by passing river waters through a system of running-water lakes accompanying the channel);

— for the Ciénaga de Tesca lagoon: at the first stage, the removal of 80% of household sewage of the town by means of construction of a centralized sewer system; at the second stage, the intensification of hydrodynamic washing of the lagoon by pure seawater by means of the construction of a system of waterworks consisting of two channels 100 m wide and a meridional jetty that originates between them; the south and the north channels connect the sea with the west and the east, respectively, parts of the basin;

— for the Ciénaga Grande de Santa Marta Firth: the construction of locks in the channels connecting the Magdalena river with the Pajarales complex of lakes and the latter with the firth for the restriction of the inflow of fresh waters into the firth in the rainy season;

— for the Odessa region of the northwest part of the Black Sea: the regulation of discharge of coastal anthropogenic sources enables one to considerably improve the ecological situation only in the regions of main discharges of waste waters (“Severnaya" and "Yuzhnaya" stations of biological purification) within the limits of the two-mile nature-conservation near-shore area; the regulation of discharge of biogenic substances by coastal sources is most efficient in the spring period; it is preferable to decrease the discharge of pollutants containing phosphorus (biogenic element), which restricts the primary production of organic matter; it is not recommended to restore the discharge from the "Severnaya" station of biological purification into the sea in the summer period; the level of trophity of waters in the marine part of the water area is formed under the dominating influence of the river discharge of the Dnieper and Yuzhnyi Bug;

— for the Tuzla group of firths: transformation into a running-water marine basin with high degree of water renewal and water quality close to that of the sea by means of construction of two channels 50 m wide at the south and north ends of the sand bay-bar spit.

The original modifications of the water-quality model presented in this work have been verified in the course of the solution of applied ecological problems for marine water areas with different morphological and operating characteristics located in different climatic zones. Methods for information support, adaptation, calibration, verification, and practical application of these models have been developed and tested. We have demonstrated information and prognostic capabilities of numerical mathematical models in the solution of applied problems of oceanology and sea ecology associated with control of water quality of ecosystems of shelf areas of the sea subject to strong anthropogenic influence.

Appendix A
Bathymetric Maps of Investigated Regions

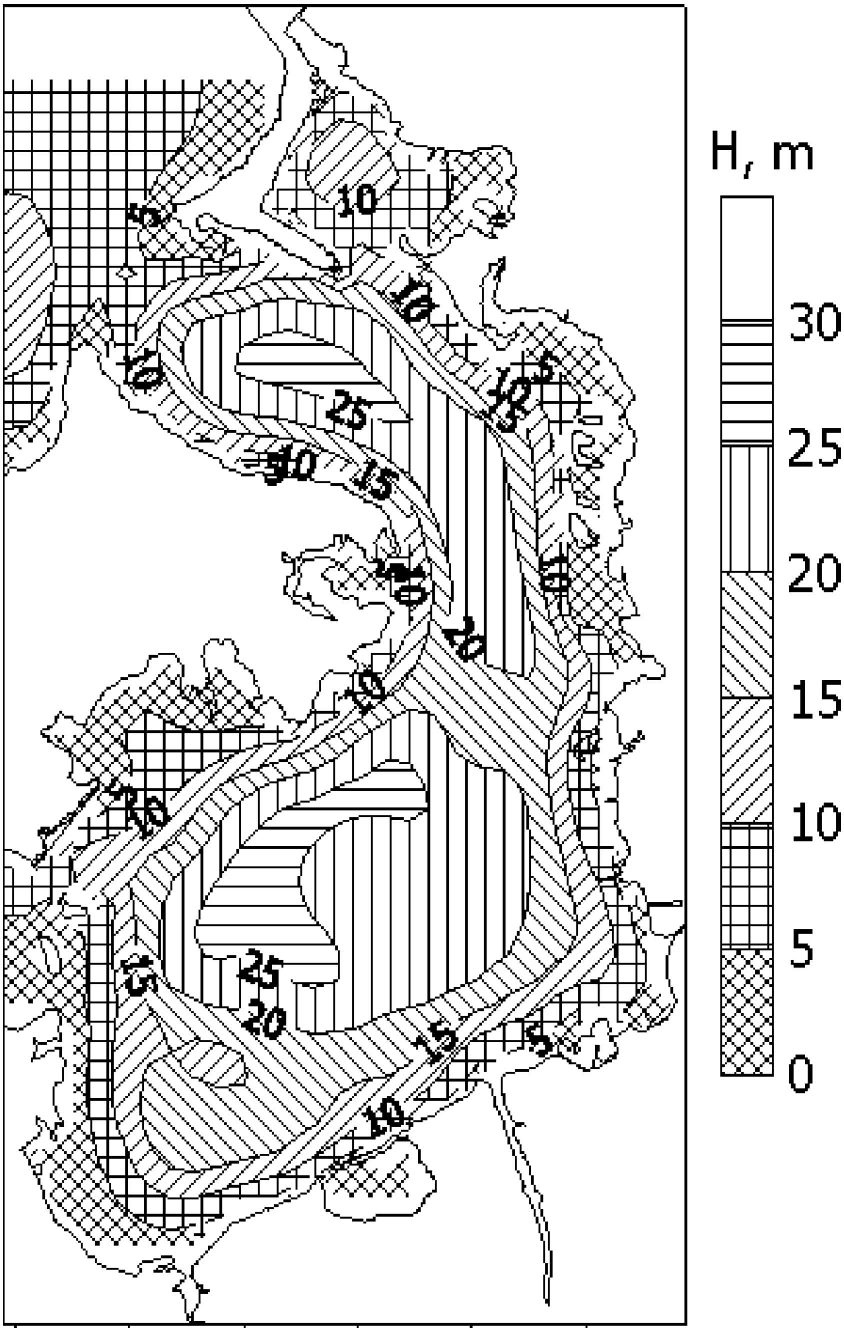


Fig. A.1. Cartagena Bay (depths in m).

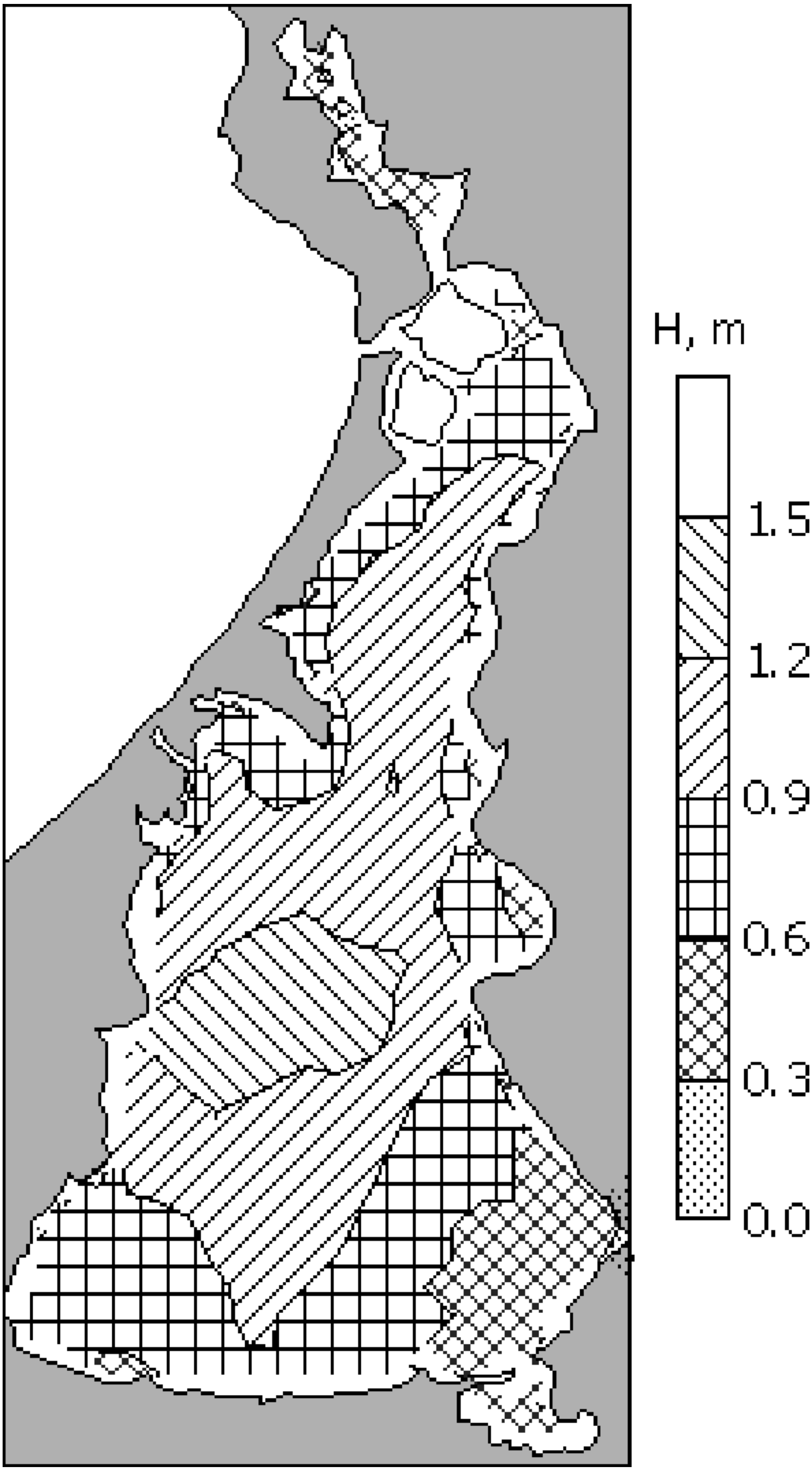


Fig. A.2. Ciénaga de Tesca Firth (depths in m).

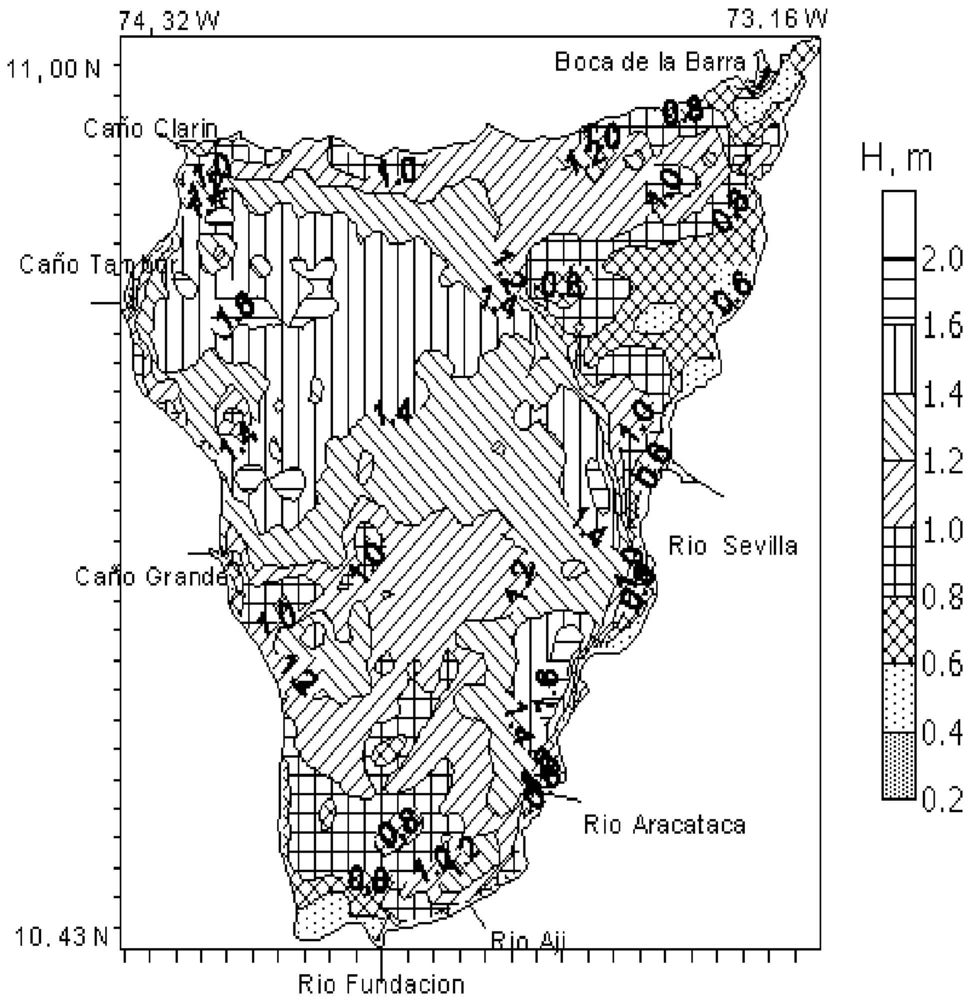


Fig. A.3. Ciénaga de Santa Marta Firth (depths in m).

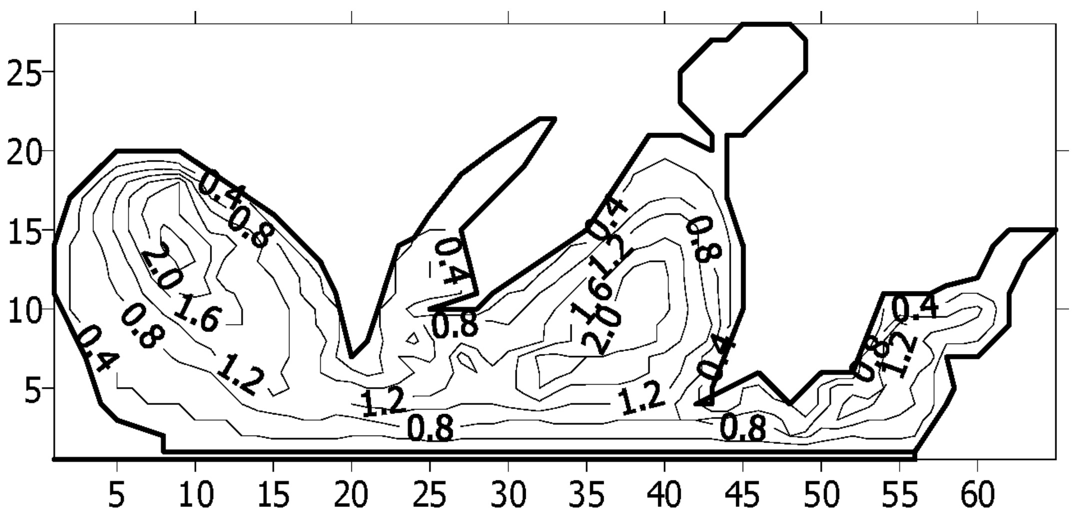


Fig. A.4. Tuzla group of firths according to the data of measurements in September, 2003 (depths in m). Space step of horizontal computational grid $\Delta x = \Delta y = 500$ m.

Appendix B
Characteristic of Anthropogenic Pollution Sources of the Investigated Marine Water Areas

Table B1. Characteristic of Waste Waters Coming to the Cartagena Bay from Industrial Objects (Fig. 2.3)

Source No.	Flow rate, m^3/day	BOD_5, kg/day	NH_4, kgN/day	NO_2, kgN/day	NO_3, kgN/day	N_{opt}, kgN/day	PO_4, kgP/day	P_{tot}, kgP/day
1	559.6	10.25	8.47	0.29	6.62	22.91	—	—
2	400.0	3171.0	225.0	—	1.74	349.40	34.11	73.36
3	800.0	98.4	7.09	0.01	0.0	36.08	3.80	5.84
4	20.0	0.114	0.01	0.01	0.01	0.052	—	0.019
5	55.0	20.30	—	—	—	0.59	—	0.24
6	87.4	102.0	—	—	—	—	—	—
7	2.8	0.01	—	—	—	—	—	—
8	984285.0	0.0	9.90	—	13.0	—	—	—
9	44.8	204.23	—	—	—	—	—	—
10	0.01	—	—	—	—	0.01	—	0.01
11	8.3	0.969	0.01	0.01	0.01	0.025	0.013	0.084
12	35.6	0.31	0.01	0.02	0.022	0.082	0.013	0.022
13	68.0	6.20	0.01	0.01	0.13	0.074	0.102	0.13
14	121089.0	1393.1	1483.5	—	—	1475.9	—	48.44
15	71.3	1.10	0.13	—	—	0.25	—	0.15
16	930.0	1.43	0.10	0.0	0.068	—	—	—
17	253200.0	0.01	0.01	0.01	0.01	0.01	0.01	0.01
18	17.3	0.02	—	—	—	—	—	—
19	6.5	0.02	—	—	—	—	—	—
20	404.8	130.34	83.46	0.01	0.01	—	—	—
21	52.6	13.15	2.31	—	—	—	—	—
22	755.1	564.05	—	—	—	14.80	—	0.54
23	19.2	10.21	0.039	0.01	0.01	0.47	—	0.02
24	33.2	0.09	0.06	—	—	0.07	0.01	0.19

Table B1 (continued)

Source No.	Flow rate, m^3/day	BOD_5, kg/day	NH_4, kgN/day	NO_2, kgN/day	NO_3, kgN/day	N_{opt}, kgN/day	PO_4, kgP/day	P_{tot}, kgP/day
25	565.9	11.45	0.07	—	—	3.04	—	5.60
26	172.8	—	0.10	—	—	4.30	—	—
27	57.7	60.31	0.30	—	—	0.37	0.39	0.50
28	54.0	29.35	—	—	—	0.59	—	0.17
29	316.0	213.93	0.32	0.03	0.02	—	—	—
Total	1364112.	6042.2	1820.9	0.41	21.65	1909.0	38.45	135.33

Table B2. Characteristic of Household Sewage Coming to the Cartagena Bay (Fig. 2.3)

Source No.	Flow rate, m^3/day	BOD_5, kg/day	NH_4, kgN/day	NO_2, kgN/day	PO_4, kgP/day	Coliforms, cell/100 ml
01	40	13.25	0.54	0.001	0.37	$125 \cdot 10^6$
02	3500	1159.2	47.14	0.098	32.44	$125 \cdot 10^6$
03	300	99.36	4.04	0.008	2.78	$125 \cdot 10^6$
04	20	6.62	0.27	0.001	0.18	$125 \cdot 10^6$
05	200	66.24	2.69	0.006	1.85	$125 \cdot 10^6$
06	150	49.68	2.02	0.004	1.39	$125 \cdot 10^6$
07	40	13.25	0.54	0.001	0.37	$125 \cdot 10^6$
10	25	8.28	0.34	0.001	0.23	$125 \cdot 10^6$
11	150	49.68	2.02	0.004	1.39	$125 \cdot 10^6$
12	100	33.12	1.35	0.003	0.93	$125 \cdot 10^6$
13	25000	8280.0	336.75	0.70	231.75	$98 \cdot 10^6$
14	1000	331.2	13.47	0.028	9.27	$98 \cdot 10^6$
16	11000	3643.2	148.17	0.308	101.97	$98 \cdot 10^6$

Table B2 (continued)

Source No.	Flow rate, m^3/day	BOD_5, kg/day	NH_4, kgN/day	NO_2, kgN/day	PO_4, kgP/day	Coliforms, cell/100 ml
17	2000	662.4	26.94	0.056	18.54	$98 \cdot 10^6$
18	2000	662.4	26.94	0.056	18.54	$98 \cdot 10^6$
Open channels	15000	1129.5	110.85	0.420	17.4	$98 \cdot 10^6$
Total	60525.0	16207.	724.1	1.70	439.4	

Table B3. Characteristic of Anthropogenic Pollution Sources of the Ciénaga de Tesca Firth (Fig. 2.7)

Source No.	Characteristic of source						
	Flow rate, m^3/day		BOD_5, kg/liter	PO_4, mgP/liter	NH_4, mgN/liter	NO, mg/liter	NO_3, mgN/liter
	1997	2025					
1	15728	38209	313.4	9.27	10.7	0.027	12.4
2	6927	7048	358.6	9.27	10.4	0.027	12.4
3	4573	6478	405.3	9.27	10.8	0.027	13.0
4	18096	20081	223.0	9.27	1.56	0.027	12.4
5	1696	2868	223.0	9.27	1.56	0.027	12.4
6	2160	2160	366.6	9.27	10.4	0.027	12.4
7	3440	6581	313.4	9.27	10.4	0.027	12.4
8.1	6357	6357	311.9	9.27	18.5	0.027	11.8
8.2	1911	1911	311.9	9.27	18.5	0.027	11.8
8.3	1845	1845	311.9	9.27	18.5	0.027	11.8
8.4	860	860	311.9	9.27	18.5	0.027	11.8
8.5	1500	1500	311.9	9.27	18.5	0.027	11.8
8.6	1500	1500	311.9	9.27	18.5	0.027	11.8
8.7	1364	1364	311.9	9.27	18.5	0.027	11.8
9	2237	6581	311.9	9.27	18.5	0.027	11.8

Table B4. Qualitative Content of Household and Industrial Sewage Discharged through Sewage Disposal Plants of the Towns of Odessa, Il'ichevsk, and Yuzhnyi

Ingredient	Odessa, "Severnaya" station of biological purification		Odessa, "Yuzhnaya" station of biological purification		Il'ichevsk and Il'ichevsk Commercial Seaport		Yuzhnyi and Odessa Harbor Plant	
	Concentration, mg/liter	Discharge in 2001, ton/yr	Concentration, mg/liter	Discharge in 2001, ton/yr	Concentration, mg/liter	Discharge in 2001, ton/yr	Concentration, mg/liter	Discharge in 2001, ton/yr
BOD_{tot}	5.20	608.90	13.60	716.70	5.73	52.11	3.60	30.50
COD	57.90	6780.00	61.50	3241.00	21.20	192.79	19.00	160.99
Oxidizability $KMnO_4$	5.10	597.20	9.91	521.70	8.50	77.30	8.80	74.56
NH_4	1.50	136.00	3.09	169.00	2.18	19.82	1.90	16.10
NO_2	0.14	12.80	0.20	11.00	0.32	2.89	0.14	1.21
NO_3	6.04	51.00	5.98	376.00	3.79	34.47	78.40	664.28
PO_4	3.04	356.00	4.52	238.00	1.990	17.28	7.90	66.94
Oil products	0.05	4.56	0.03	1.53	0.04	0.39	0.10	0.85

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